



# wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 01:05 PM UTC

PDB ID : 8WMJ / pdb\_00008wmj  
EMDB ID : EMD-37654  
Title : structure of PSI-11CAC complex at Logarithmic growth phase  
Authors : Zhang, S.M.; Si, L.; Li, M.  
Deposited on : 2023-10-03  
Resolution : 3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

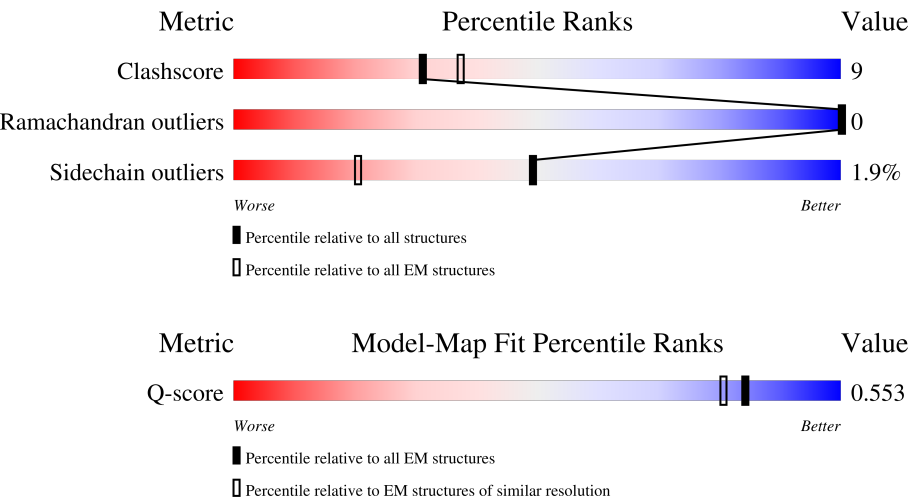
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



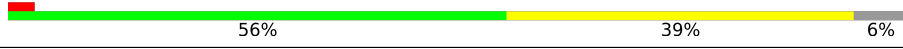
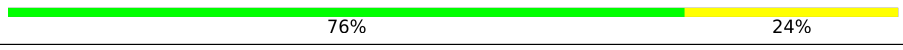
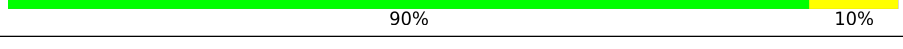
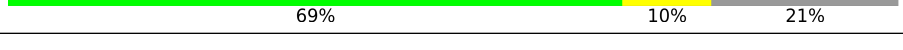
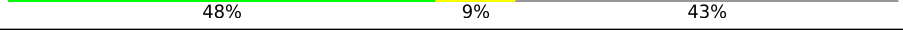
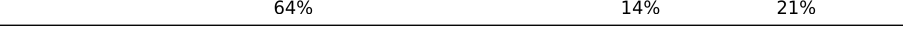
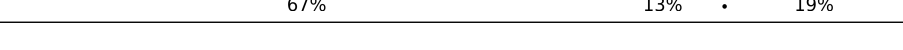
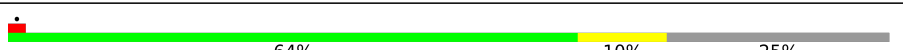
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14081 ( 2.50 - 3.50 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                |
|-----|-------|--------|-----------------------------------------------------------------|
| 1   | A     | 752    | <div><div></div><div>84%</div><div>14%</div><div>.</div></div>  |
| 2   | B     | 734    | <div><div></div><div>83%</div><div>16%</div><div></div></div>   |
| 3   | C     | 81     | <div><div></div><div>73%</div><div>22%</div><div>..</div></div> |
| 4   | D     | 141    | <div><div></div><div>77%</div><div>20%</div><div>..</div></div> |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | E     | 64     |    |
| 6   | F     | 188    |    |
| 7   | I     | 36     |    |
| 8   | J     | 42     |    |
| 9   | L     | 153    |    |
| 10  | M     | 30     |    |
| 11  | K     | 87     |    |
| 12  | s     | 269    |    |
| 13  | c     | 216    |    |
| 14  | a     | 216    |    |
| 15  | b     | 223    |    |
| 16  | h     | 225    |  |
| 17  | j     | 212    |  |
| 17  | m     | 212    |  |
| 18  | l     | 238    |  |
| 19  | k     | 241    |  |
| 20  | i     | 218    |  |
| 21  | d     | 213    |  |
| 22  | R     | 129    |  |
| 23  | n     | 219    |  |
| 24  | Q     | 234    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | A     | 801 | X         | -        | -       | -                |
| 25  | CLA  | A     | 802 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | A     | 804 | X         | -        | -       | -                |
| 25  | CLA  | A     | 805 | X         | -        | -       | -                |
| 25  | CLA  | A     | 807 | X         | -        | -       | -                |
| 25  | CLA  | A     | 808 | X         | -        | -       | -                |
| 25  | CLA  | A     | 810 | X         | -        | -       | -                |
| 25  | CLA  | A     | 812 | X         | -        | -       | -                |
| 25  | CLA  | A     | 817 | X         | -        | -       | -                |
| 25  | CLA  | A     | 818 | X         | -        | -       | -                |
| 25  | CLA  | A     | 820 | X         | -        | -       | -                |
| 25  | CLA  | A     | 824 | X         | -        | -       | -                |
| 25  | CLA  | A     | 826 | X         | -        | -       | -                |
| 25  | CLA  | A     | 829 | X         | -        | -       | -                |
| 25  | CLA  | A     | 833 | X         | -        | -       | -                |
| 25  | CLA  | A     | 834 | X         | -        | -       | -                |
| 25  | CLA  | A     | 835 | X         | -        | -       | -                |
| 25  | CLA  | A     | 837 | X         | -        | -       | -                |
| 25  | CLA  | A     | 838 | X         | -        | -       | -                |
| 25  | CLA  | A     | 839 | X         | -        | -       | -                |
| 25  | CLA  | A     | 841 | X         | -        | -       | -                |
| 25  | CLA  | A     | 842 | X         | -        | -       | -                |
| 25  | CLA  | A     | 843 | X         | -        | -       | -                |
| 25  | CLA  | A     | 853 | X         | -        | -       | -                |
| 25  | CLA  | A     | 854 | X         | -        | -       | -                |
| 25  | CLA  | A     | 855 | X         | -        | -       | -                |
| 25  | CLA  | A     | 856 | X         | -        | -       | -                |
| 25  | CLA  | B     | 803 | X         | -        | -       | -                |
| 25  | CLA  | B     | 804 | X         | -        | -       | -                |
| 25  | CLA  | B     | 805 | X         | -        | -       | -                |
| 25  | CLA  | B     | 806 | X         | -        | -       | -                |
| 25  | CLA  | B     | 807 | X         | -        | -       | -                |
| 25  | CLA  | B     | 808 | X         | -        | -       | -                |
| 25  | CLA  | B     | 809 | X         | -        | -       | -                |
| 25  | CLA  | B     | 810 | X         | -        | -       | -                |
| 25  | CLA  | B     | 811 | X         | -        | -       | -                |
| 25  | CLA  | B     | 812 | X         | -        | -       | -                |
| 25  | CLA  | B     | 813 | X         | -        | -       | -                |
| 25  | CLA  | B     | 814 | X         | -        | -       | -                |
| 25  | CLA  | B     | 816 | X         | -        | -       | -                |
| 25  | CLA  | B     | 817 | X         | -        | -       | -                |
| 25  | CLA  | B     | 818 | X         | -        | -       | -                |
| 25  | CLA  | B     | 822 | X         | -        | -       | -                |
| 25  | CLA  | B     | 824 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | B     | 825 | X         | -        | -       | -                |
| 25  | CLA  | B     | 826 | X         | -        | -       | -                |
| 25  | CLA  | B     | 832 | X         | -        | -       | -                |
| 25  | CLA  | B     | 833 | X         | -        | -       | -                |
| 25  | CLA  | B     | 834 | X         | -        | -       | -                |
| 25  | CLA  | B     | 835 | X         | -        | -       | -                |
| 25  | CLA  | B     | 837 | X         | -        | -       | -                |
| 25  | CLA  | B     | 839 | X         | -        | -       | -                |
| 25  | CLA  | B     | 840 | X         | -        | -       | -                |
| 25  | CLA  | B     | 841 | X         | -        | -       | -                |
| 25  | CLA  | B     | 850 | X         | -        | -       | -                |
| 25  | CLA  | F     | 201 | X         | -        | -       | -                |
| 25  | CLA  | J     | 103 | X         | -        | -       | -                |
| 25  | CLA  | K     | 101 | X         | -        | -       | -                |
| 25  | CLA  | K     | 102 | X         | -        | -       | -                |
| 25  | CLA  | L     | 202 | X         | -        | -       | -                |
| 25  | CLA  | Q     | 302 | X         | -        | -       | -                |
| 25  | CLA  | Q     | 303 | X         | -        | -       | -                |
| 25  | CLA  | R     | 202 | X         | -        | -       | -                |
| 25  | CLA  | a     | 303 | X         | -        | -       | -                |
| 25  | CLA  | a     | 304 | X         | -        | -       | -                |
| 25  | CLA  | a     | 305 | X         | -        | -       | -                |
| 25  | CLA  | a     | 306 | X         | -        | -       | -                |
| 25  | CLA  | a     | 308 | X         | -        | -       | -                |
| 25  | CLA  | a     | 309 | X         | -        | -       | -                |
| 25  | CLA  | a     | 310 | X         | -        | -       | -                |
| 25  | CLA  | a     | 311 | X         | -        | -       | -                |
| 25  | CLA  | a     | 313 | X         | -        | -       | -                |
| 25  | CLA  | b     | 601 | X         | -        | -       | -                |
| 25  | CLA  | b     | 602 | X         | -        | -       | -                |
| 25  | CLA  | b     | 603 | X         | -        | -       | -                |
| 25  | CLA  | b     | 605 | X         | -        | -       | -                |
| 25  | CLA  | b     | 606 | X         | -        | -       | -                |
| 25  | CLA  | b     | 607 | X         | -        | -       | -                |
| 25  | CLA  | b     | 608 | X         | -        | -       | -                |
| 25  | CLA  | b     | 610 | X         | -        | -       | -                |
| 25  | CLA  | b     | 611 | X         | -        | -       | -                |
| 25  | CLA  | c     | 601 | X         | -        | -       | -                |
| 25  | CLA  | c     | 602 | X         | -        | -       | -                |
| 25  | CLA  | c     | 603 | X         | -        | -       | -                |
| 25  | CLA  | c     | 604 | X         | -        | -       | -                |
| 25  | CLA  | c     | 605 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | c     | 607 | X         | -        | -       | -                |
| 25  | CLA  | c     | 608 | X         | -        | -       | -                |
| 25  | CLA  | c     | 609 | X         | -        | -       | -                |
| 25  | CLA  | c     | 612 | X         | -        | -       | -                |
| 25  | CLA  | d     | 301 | X         | -        | -       | -                |
| 25  | CLA  | d     | 302 | X         | -        | -       | -                |
| 25  | CLA  | d     | 303 | X         | -        | -       | -                |
| 25  | CLA  | d     | 304 | X         | -        | -       | -                |
| 25  | CLA  | d     | 305 | X         | -        | -       | -                |
| 25  | CLA  | d     | 306 | X         | -        | -       | -                |
| 25  | CLA  | d     | 307 | X         | -        | -       | -                |
| 25  | CLA  | d     | 308 | X         | -        | -       | -                |
| 25  | CLA  | d     | 309 | X         | -        | -       | -                |
| 25  | CLA  | d     | 312 | X         | -        | -       | -                |
| 25  | CLA  | h     | 302 | X         | -        | -       | -                |
| 25  | CLA  | h     | 303 | X         | -        | -       | -                |
| 25  | CLA  | h     | 304 | X         | -        | -       | -                |
| 25  | CLA  | h     | 305 | X         | -        | -       | -                |
| 25  | CLA  | h     | 306 | X         | -        | -       | -                |
| 25  | CLA  | h     | 307 | X         | -        | -       | -                |
| 25  | CLA  | h     | 308 | X         | -        | -       | -                |
| 25  | CLA  | h     | 313 | X         | -        | -       | -                |
| 25  | CLA  | i     | 302 | X         | -        | -       | -                |
| 25  | CLA  | i     | 303 | X         | -        | -       | -                |
| 25  | CLA  | i     | 304 | X         | -        | -       | -                |
| 25  | CLA  | i     | 306 | X         | -        | -       | -                |
| 25  | CLA  | i     | 307 | X         | -        | -       | -                |
| 25  | CLA  | i     | 308 | X         | -        | -       | -                |
| 25  | CLA  | i     | 309 | X         | -        | -       | -                |
| 25  | CLA  | i     | 311 | X         | -        | -       | -                |
| 25  | CLA  | i     | 312 | X         | -        | -       | -                |
| 25  | CLA  | j     | 601 | X         | -        | -       | -                |
| 25  | CLA  | j     | 603 | X         | -        | -       | -                |
| 25  | CLA  | j     | 605 | X         | -        | -       | -                |
| 25  | CLA  | j     | 606 | X         | -        | -       | -                |
| 25  | CLA  | j     | 607 | X         | -        | -       | -                |
| 25  | CLA  | j     | 608 | X         | -        | -       | -                |
| 25  | CLA  | j     | 609 | X         | -        | -       | -                |
| 25  | CLA  | j     | 611 | X         | -        | -       | -                |
| 25  | CLA  | j     | 612 | X         | -        | -       | -                |
| 25  | CLA  | k     | 601 | X         | -        | -       | -                |
| 25  | CLA  | k     | 602 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | k     | 603 | X         | -        | -       | -                |
| 25  | CLA  | k     | 605 | X         | -        | -       | -                |
| 25  | CLA  | k     | 607 | X         | -        | -       | -                |
| 25  | CLA  | k     | 608 | X         | -        | -       | -                |
| 25  | CLA  | k     | 609 | X         | -        | -       | -                |
| 25  | CLA  | k     | 610 | X         | -        | -       | -                |
| 25  | CLA  | l     | 303 | X         | -        | -       | -                |
| 25  | CLA  | l     | 304 | X         | -        | -       | -                |
| 25  | CLA  | l     | 305 | X         | -        | -       | -                |
| 25  | CLA  | l     | 307 | X         | -        | -       | -                |
| 25  | CLA  | l     | 308 | X         | -        | -       | -                |
| 25  | CLA  | l     | 309 | X         | -        | -       | -                |
| 25  | CLA  | l     | 310 | X         | -        | -       | -                |
| 25  | CLA  | l     | 312 | X         | -        | -       | -                |
| 25  | CLA  | m     | 601 | X         | -        | -       | -                |
| 25  | CLA  | m     | 602 | X         | -        | -       | -                |
| 25  | CLA  | m     | 603 | X         | -        | -       | -                |
| 25  | CLA  | m     | 606 | X         | -        | -       | -                |
| 25  | CLA  | m     | 608 | X         | -        | -       | -                |
| 25  | CLA  | m     | 609 | X         | -        | -       | -                |
| 25  | CLA  | m     | 610 | X         | -        | -       | -                |
| 25  | CLA  | m     | 613 | X         | -        | -       | -                |
| 25  | CLA  | n     | 302 | X         | -        | -       | -                |
| 25  | CLA  | n     | 303 | X         | -        | -       | -                |
| 25  | CLA  | n     | 304 | X         | -        | -       | -                |
| 25  | CLA  | n     | 305 | X         | -        | -       | -                |
| 25  | CLA  | n     | 306 | X         | -        | -       | -                |
| 25  | CLA  | n     | 307 | X         | -        | -       | -                |
| 25  | CLA  | n     | 308 | X         | -        | -       | -                |
| 25  | CLA  | n     | 309 | X         | -        | -       | -                |
| 25  | CLA  | n     | 310 | X         | -        | -       | -                |
| 25  | CLA  | s     | 202 | X         | -        | -       | -                |
| 25  | CLA  | s     | 209 | X         | -        | -       | -                |
| 30  | SF4  | B     | 802 | -         | -        | X       | -                |
| 30  | SF4  | C     | 102 | -         | -        | X       | -                |

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 52744 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 1   | A     | 742      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5825  | 3802 | 994 | 1001 | 28 |         |       |

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 732      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5820  | 3840 | 981 | 984 | 15 |         |       |

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | C     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 592   | 361 | 103 | 116 | 12 |         |       |

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1084  | 692 | 186 | 203 | 3 |         |       |

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 5   | E     | 60       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 485   | 309 | 84 | 92 |         |       |

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1254  | 814 | 212 | 226 | 2 |         |       |

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | I     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 264   | 182 | 35 | 45 | 2 |         |       |

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | J     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 351   | 240 | 49 | 59 | 3 |         |       |

- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | L     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1146  | 753 | 182 | 208 | 3 |         |       |

- Molecule 10 is a protein called Photosystem I reaction center subunit XII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | M     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 232   | 155 | 38 | 38 | 1 |         |       |

- Molecule 11 is a protein called Photosystem I reaction center subunit PsaK.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | K     | 69       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 488   | 319 | 80 | 87 | 2 |         |       |

- Molecule 12 is a protein called chain s.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | s     | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1140  | 719 | 195 | 217 | 9 |         |       |

- Molecule 13 is a protein called CAC-c.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | c     | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1357  | 897 | 221 | 236 | 3 |         |       |

- Molecule 14 is a protein called CAC-a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 14  | a     | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1361  | 889 | 217 | 245 | 10 |         |       |

- Molecule 15 is a protein called CAC-b.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 15  | b     | 194      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1439  | 916 | 251 | 258 | 14 |         |       |

- Molecule 16 is a protein called CAC-h.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | h     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1200  | 778 | 202 | 214 | 6 |         |       |

- Molecule 17 is a protein called CAC-j.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | m     | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1309  | 846 | 214 | 241 | 8 |         |       |
| 17  | j     | 172      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1293  | 834 | 212 | 239 | 8 |         |       |

- Molecule 18 is a protein called CAC-l.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | l     | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1344  | 869 | 230 | 238 | 7 |         |       |

- Molecule 19 is a protein called CAC-k.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 19  | k     | 180      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1346  | 872 | 223 | 239 | 12 |         |       |

- Molecule 20 is a protein called CAC-i.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 20  | i     | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1324  | 849 | 227 | 237 | 11 |         |       |

- Molecule 21 is a protein called CAC-d.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 21  | d     | 129      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 974   | 624 | 169 | 171 | 10 |         |       |

- Molecule 22 is a protein called PsaR.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | R     | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 664   | 434 | 105 | 124 | 1 |         |       |

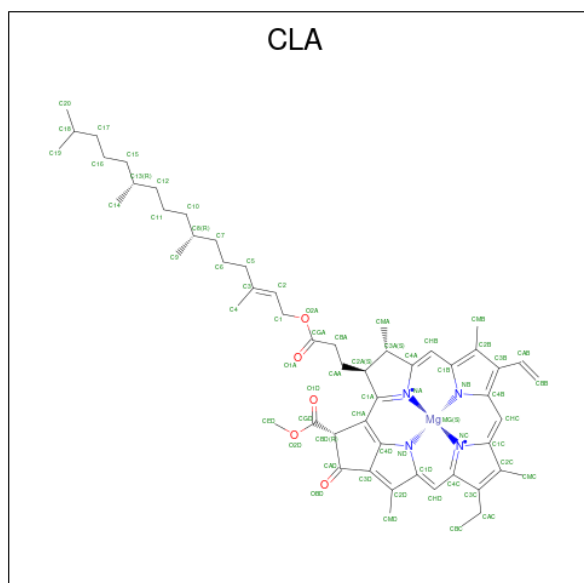
- Molecule 23 is a protein called CAC-n.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23  | n     | 181      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1350  | 870 | 228 | 242 | 10 |         |       |

- Molecule 24 is a protein called PsaQ.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | Q     | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1226  | 775 | 208 | 238 | 5 |         |       |

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 25  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | A     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 53    | 43 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 54 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 47 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | F     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | F     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | J     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 25  | L     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | L     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | K     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | K     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 25  | s     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | s     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | s     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | s     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | h     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | h     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | h     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | h     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | h     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | h     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | h     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | h     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | h     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | m     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 25  | m     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | m     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | m     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | m     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 25  | m     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | m     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | m     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | m     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | m     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | m     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | m     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 25  | l     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | l     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | l     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | l     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | l     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | l     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | l     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | l     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | l     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | l     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | k     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | k     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | k     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | k     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | k     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | k     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | k     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | k     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | k     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | k     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | k     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | i     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | i     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | i     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | i     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | i     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | i     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | i     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | i     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | i     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | i     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | j     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | j     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | j     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | j     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | j     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | j     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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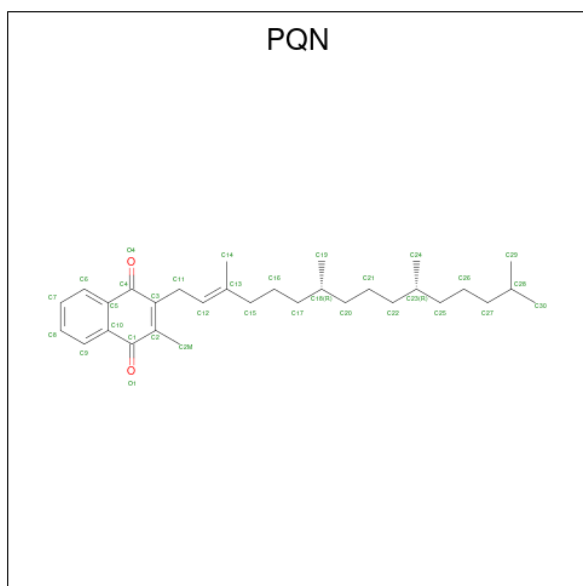
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | j     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | j     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | j     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | j     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | j     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | d     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | d     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | d     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | d     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | d     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | d     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | d     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | d     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 25  | d     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 25  | d     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | R     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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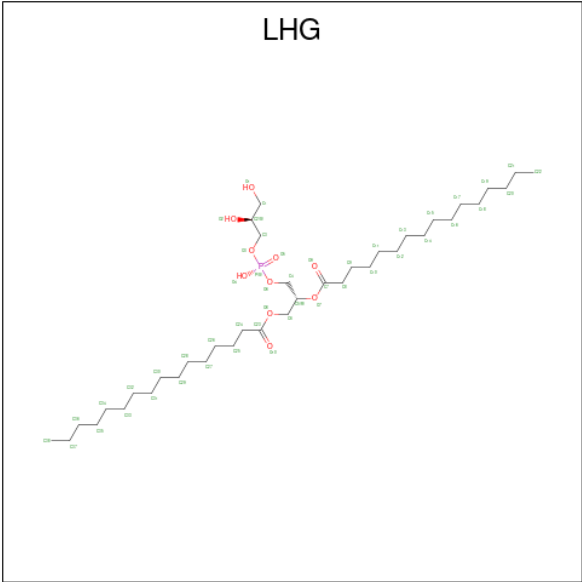
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 25  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 25  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 25  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | Q     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | Q     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 26  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 26  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



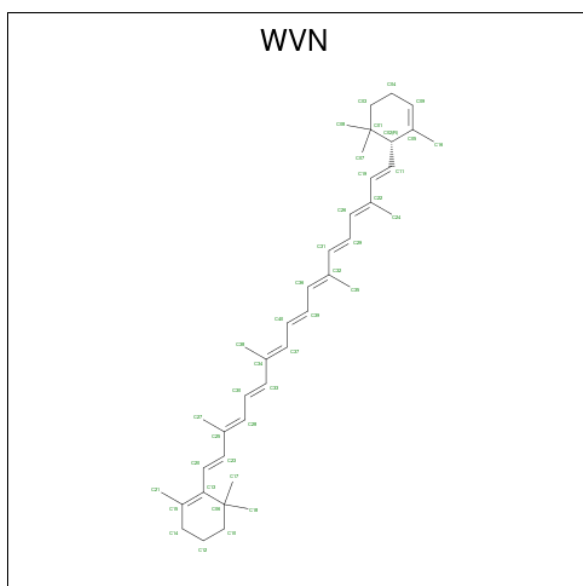
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 27  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 48    | 37 | 10 | 1 |         |
| 27  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 27    | 16 | 10 | 1 |         |
| 27  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 38    | 27 | 10 | 1 |         |
| 27  | J     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 27  | J     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 31    | 20 | 10 | 1 |         |
| 27  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 27  | c     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 27  | c     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 27  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 27  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 27  | b     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 27  | m     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 27  | l     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 32    | 21 | 10 | 1 |         |
| 27  | k     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |

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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 27  | i     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 27  | j     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 30    | 19 | 10 | 1 |         |
| 27  | d     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 27  | n     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |

- Molecule 28 is 1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene (CCD ID: WVN) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 28  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

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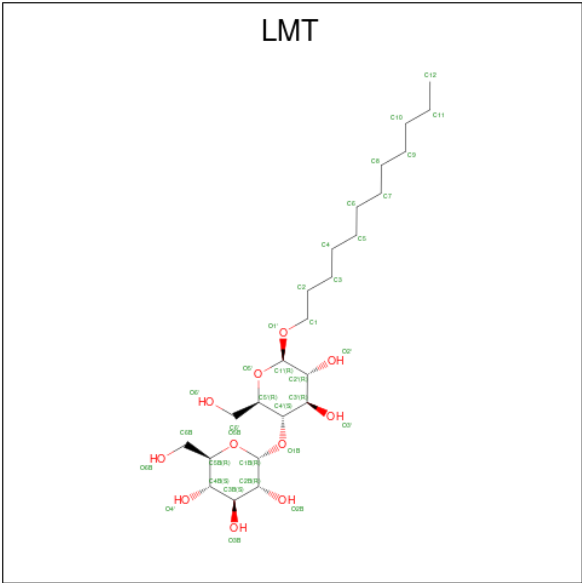
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 28  | B     | 1        | Total C<br>40 40 | 0       |
| 28  | B     | 1        | Total C<br>40 40 | 0       |
| 28  | B     | 1        | Total C<br>40 40 | 0       |
| 28  | B     | 1        | Total C<br>40 40 | 0       |
| 28  | B     | 1        | Total C<br>40 40 | 0       |
| 28  | F     | 1        | Total C<br>40 40 | 0       |
| 28  | F     | 1        | Total C<br>40 40 | 0       |
| 28  | I     | 1        | Total C<br>40 40 | 0       |
| 28  | J     | 1        | Total C<br>40 40 | 0       |
| 28  | J     | 1        | Total C<br>40 40 | 0       |
| 28  | L     | 1        | Total C<br>40 40 | 0       |
| 28  | L     | 1        | Total C<br>40 40 | 0       |
| 28  | L     | 1        | Total C<br>40 40 | 0       |
| 28  | M     | 1        | Total C<br>40 40 | 0       |
| 28  | K     | 1        | Total C<br>40 40 | 0       |
| 28  | s     | 1        | Total C<br>40 40 | 0       |
| 28  | s     | 1        | Total C<br>40 40 | 0       |
| 28  | h     | 1        | Total C<br>40 40 | 0       |
| 28  | l     | 1        | Total C<br>40 40 | 0       |
| 28  | l     | 1        | Total C<br>40 40 | 0       |
| 28  | i     | 1        | Total C<br>40 40 | 0       |

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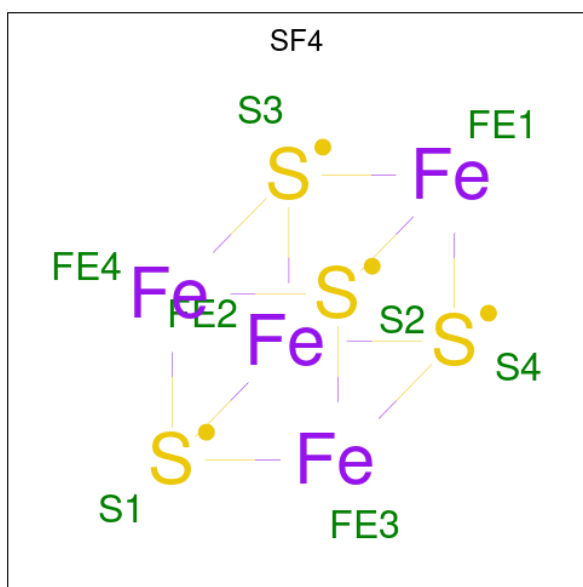
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 28  | R     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

- Molecule 29 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



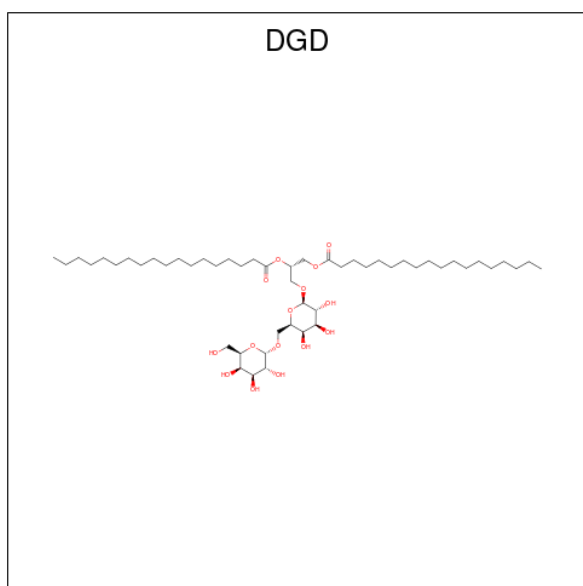
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 29  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 29  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 24    | 18 | 6  |         |
| 29  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 29  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 24    | 18 | 6  |         |

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



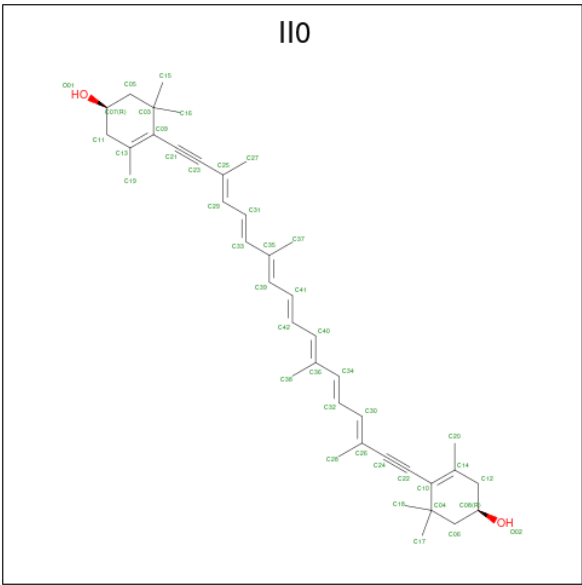
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 30  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 30  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 30  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 31  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 60    | 45 | 15 |         |

- Molecule 32 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 32  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

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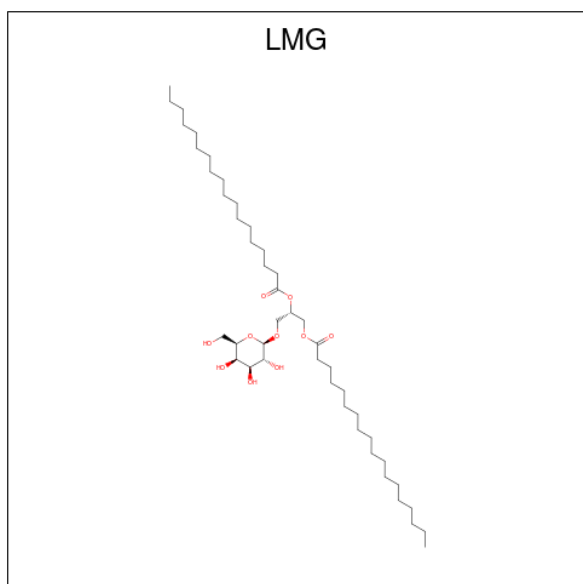
| Mol | Chain | Residues | Atoms       |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|
| 32  | b     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | b     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | h     | 1        | Total<br>28 | C<br>27 | O<br>1 | 0       |
| 32  | h     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | h     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | m     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | m     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | m     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | l     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | l     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | l     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | l     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | l     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | k     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | k     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | k     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | k     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | i     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | i     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | i     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | i     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 32  | i     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |

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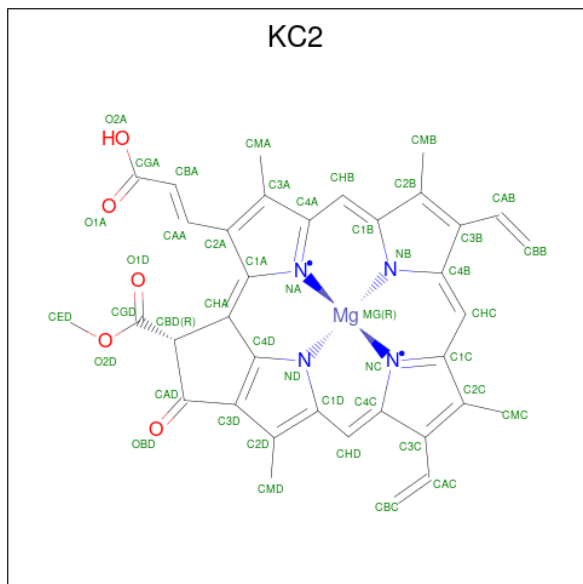
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 32  | j     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | j     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | j     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 32  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



| Mol | Chain | Residues | Atoms       |         |         | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 33  | J     | 1        | Total<br>55 | C<br>45 | O<br>10 | 0       |
| 33  | s     | 1        | Total<br>48 | C<br>38 | O<br>10 | 0       |
| 33  | c     | 1        | Total<br>55 | C<br>45 | O<br>10 | 0       |
| 33  | b     | 1        | Total<br>49 | C<br>39 | O<br>10 | 0       |
| 33  | n     | 1        | Total<br>55 | C<br>45 | O<br>10 | 0       |
| 33  | Q     | 1        | Total<br>38 | C<br>28 | O<br>10 | 0       |

- Molecule 34 is Chlorophyll c2 (CCD ID: KC2) (formula:  $C_{35}H_{28}MgN_4O_5$ ).



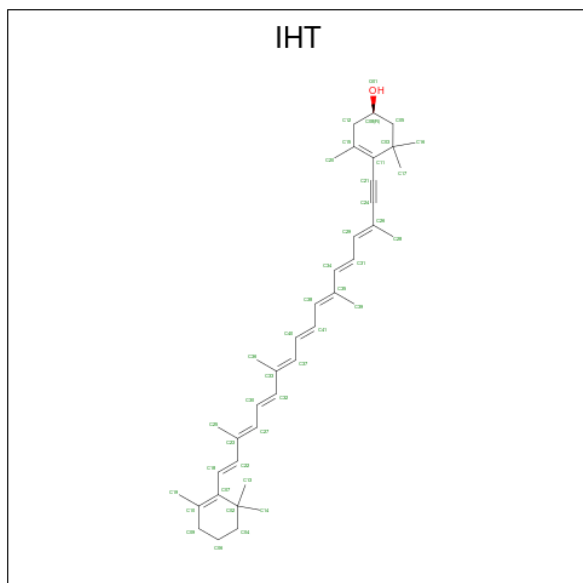
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 34  | s     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 34  | s     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 34  | c     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 34  | m     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 34  | l     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 34  | k     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 34  | k     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 34  | k     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 34  | i     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 34  | i     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 34  | j     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 34  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 34  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 34  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 34  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

- Molecule 35 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: C<sub>40</sub>H<sub>54</sub>O).



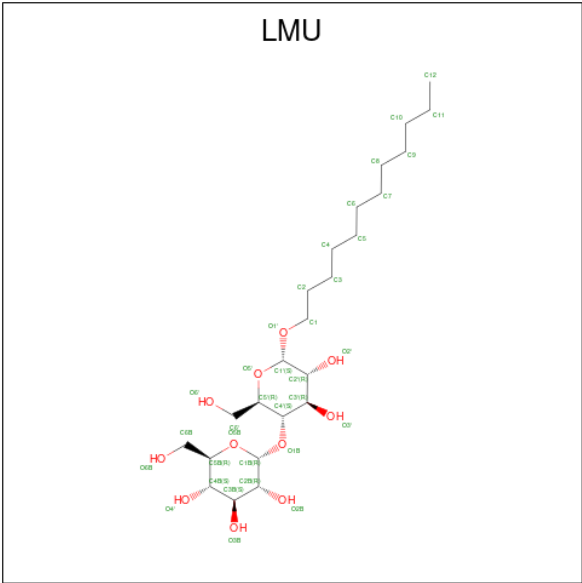
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 35  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 35  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 35  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 35  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 35  | m     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 35  | k     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 35  | j     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 35  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 35  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |

- Molecule 36 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 36  | i     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

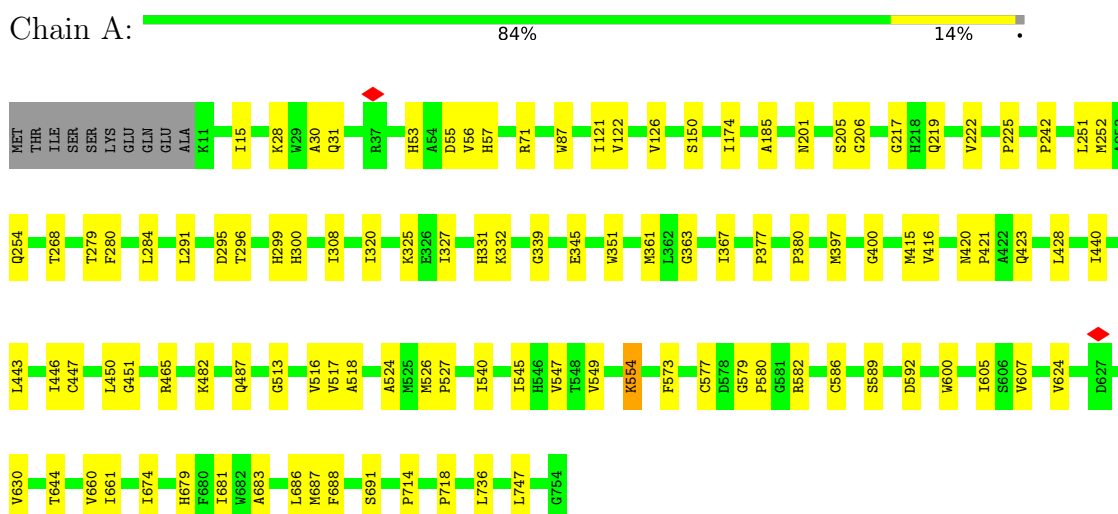
- Molecule 37 is water.

| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 37  | A     | 48       | Total<br>48 | O<br>48 | 0       |
| 37  | B     | 58       | Total<br>58 | O<br>58 | 0       |
| 37  | C     | 8        | Total<br>8  | O<br>8  | 0       |
| 37  | D     | 1        | Total<br>1  | O<br>1  | 0       |
| 37  | F     | 3        | Total<br>3  | O<br>3  | 0       |
| 37  | I     | 1        | Total<br>1  | O<br>1  | 0       |
| 37  | J     | 1        | Total<br>1  | O<br>1  | 0       |
| 37  | L     | 1        | Total<br>1  | O<br>1  | 0       |
| 37  | K     | 1        | Total<br>1  | O<br>1  | 0       |
| 37  | a     | 3        | Total<br>3  | O<br>3  | 0       |
| 37  | b     | 2        | Total<br>2  | O<br>2  | 0       |
| 37  | h     | 1        | Total<br>1  | O<br>1  | 0       |
| 37  | m     | 1        | Total<br>1  | O<br>1  | 0       |
| 37  | R     | 1        | Total<br>1  | O<br>1  | 0       |
| 37  | n     | 2        | Total<br>2  | O<br>2  | 0       |
| 37  | Q     | 1        | Total<br>1  | O<br>1  | 0       |

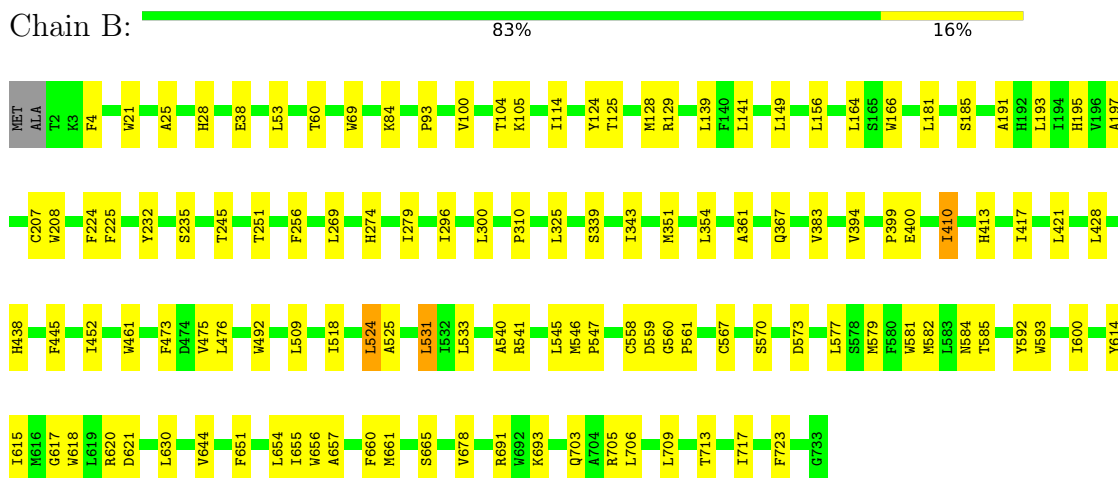
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

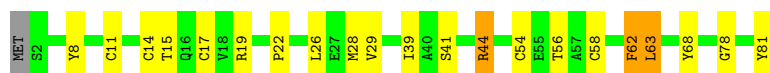


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center





- Molecule 4: Photosystem I reaction center subunit II

Chain D: 77% 20% ..



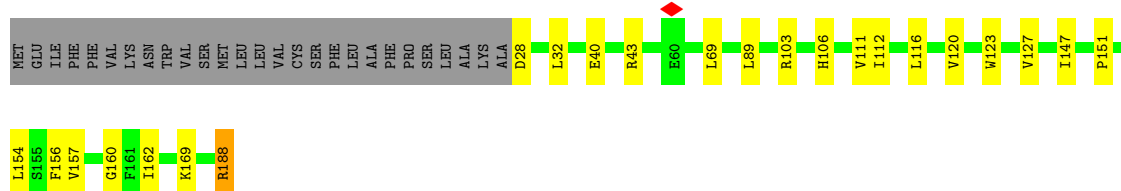
- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 80% 14% 6%



- Molecule 6: Photosystem I reaction center subunit III

Chain F: 73% 12% 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 56% 39% 6%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 76% 24%



- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 89% 10%





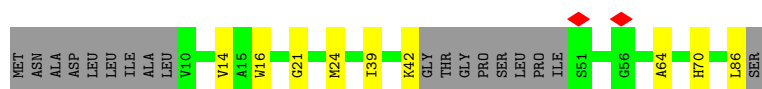
- Molecule 10: Photosystem I reaction center subunit XII

Chain M:  90% 10%

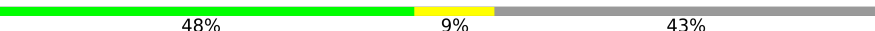


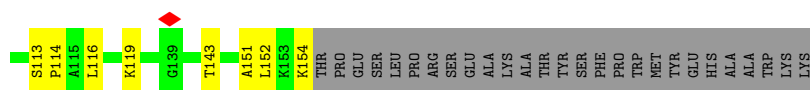
- Molecule 11: Photosystem I reaction center subunit PsaK

Chain K:  69% 10% 21%



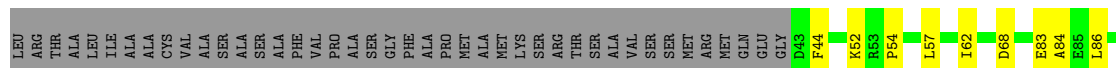
- Molecule 12: chain s

Chain s:  48% 9% 43%



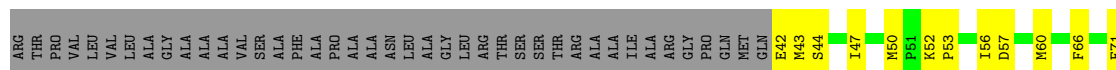
- Molecule 13: CAC-c

Chain c:  64% 14% 21%



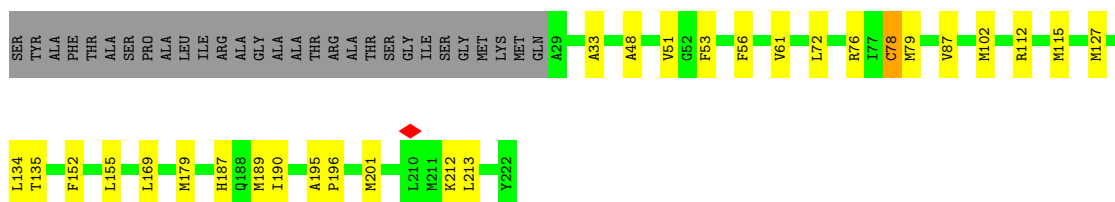
- Molecule 14: CAC-a

Chain a:  67% 13% 19%

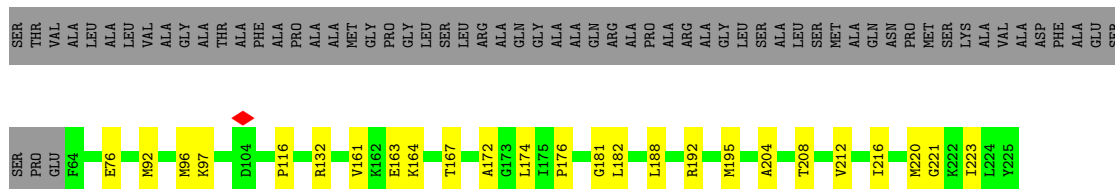


- Molecule 15: CAC-b

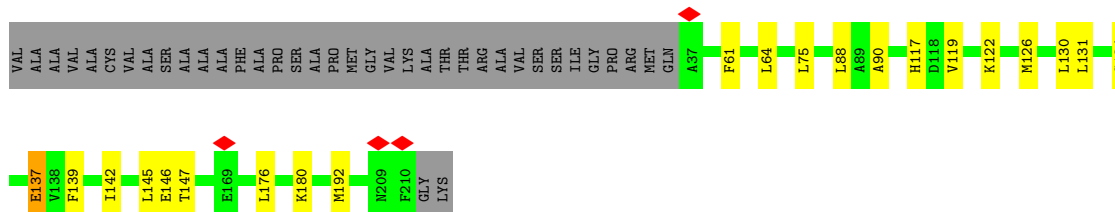
Chain b:  74% 13% 13%



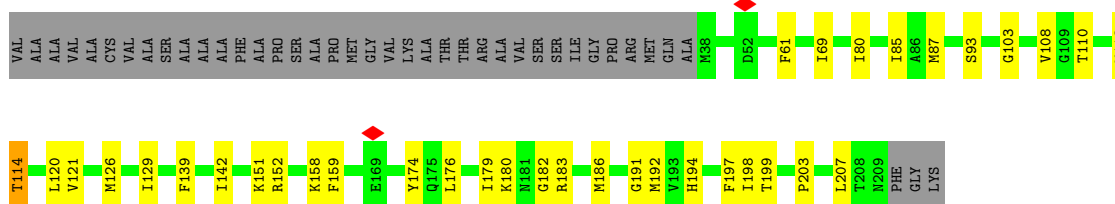
• Molecule 16: CAC-h



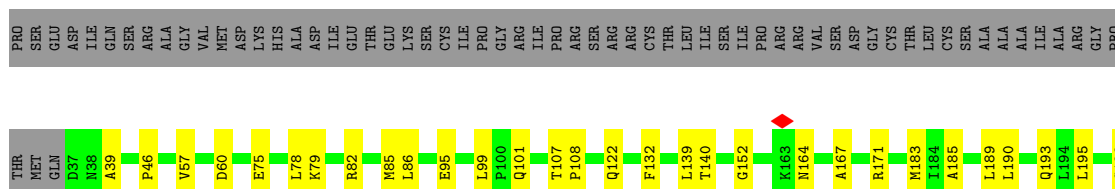
• Molecule 17: CAC-j



• Molecule 17: CAC-j

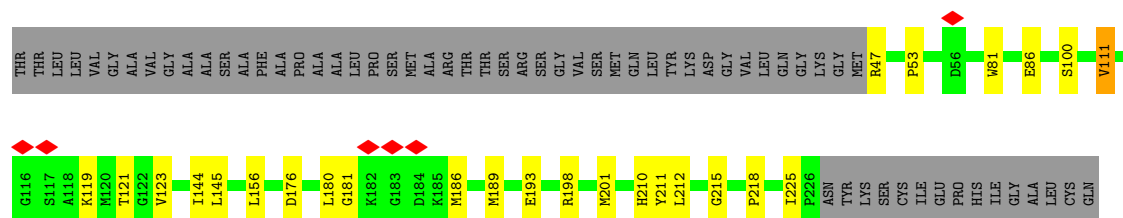


• Molecule 18: CAC-l

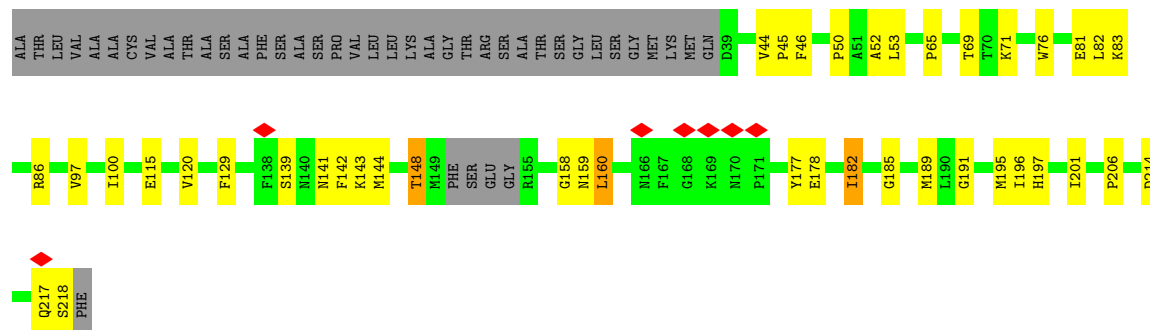




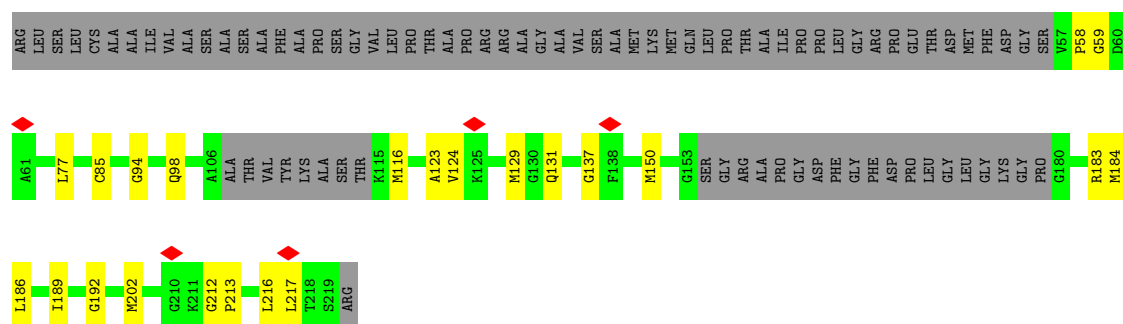
- Molecule 19: CAC-k



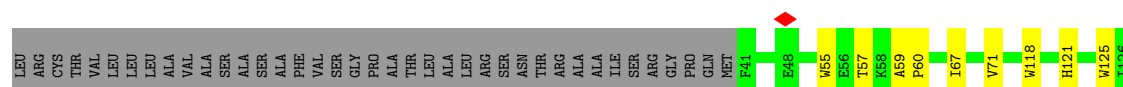
- Molecule 20: CAC-i



- Molecule 21: CAC-d



- Molecule 22: Psar

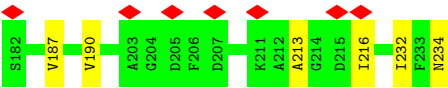
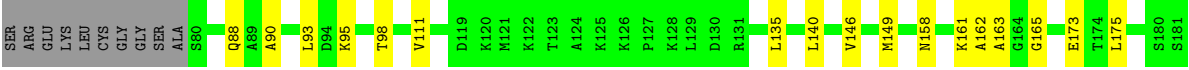
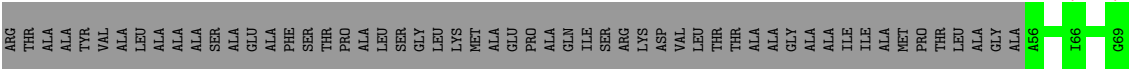




• Molecule 23: CAC-n



• Molecule 24: PsaQ



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 41093                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TALOS ARCTICA                       | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 2200                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k)              | Depositor |
| Maximum map value                    | 0.265                                   | Depositor |
| Minimum map value                    | -0.145                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.02                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 360.0, 360.0, 360.0                     | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.0, 1.0, 1.0                           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHT, LMG, DGD, WVN, LMT, SF4, LMU, KC2, II0, PQN, LHG, CLA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.52         | 0/6019  | 0.70        | 0/8204         |
| 2   | B     | 0.57         | 0/6036  | 0.80        | 0/8242         |
| 3   | C     | 0.70         | 0/601   | 1.02        | 1/813 (0.1%)   |
| 4   | D     | 0.52         | 0/1109  | 0.80        | 0/1500         |
| 5   | E     | 0.66         | 0/493   | 0.83        | 0/667          |
| 6   | F     | 0.49         | 0/1287  | 0.73        | 0/1747         |
| 7   | I     | 0.77         | 0/271   | 1.01        | 0/370          |
| 8   | J     | 0.41         | 0/364   | 0.70        | 0/495          |
| 9   | L     | 0.45         | 0/1175  | 0.78        | 0/1599         |
| 10  | M     | 0.36         | 0/233   | 0.87        | 2/315 (0.6%)   |
| 11  | K     | 0.60         | 0/495   | 0.92        | 0/672          |
| 12  | s     | 0.58         | 0/1170  | 0.85        | 0/1580         |
| 13  | c     | 0.50         | 0/1396  | 0.79        | 0/1889         |
| 14  | a     | 0.53         | 0/1406  | 0.81        | 0/1903         |
| 15  | b     | 0.54         | 0/1469  | 0.84        | 0/1983         |
| 16  | h     | 0.44         | 0/1226  | 0.73        | 0/1667         |
| 17  | j     | 0.61         | 0/1318  | 0.95        | 1/1775 (0.1%)  |
| 17  | m     | 0.53         | 0/1335  | 0.81        | 0/1798         |
| 18  | l     | 0.51         | 0/1379  | 0.83        | 0/1863         |
| 19  | k     | 0.61         | 0/1380  | 0.90        | 0/1869         |
| 20  | i     | 0.63         | 0/1359  | 0.97        | 0/1835         |
| 21  | d     | 0.68         | 0/993   | 1.00        | 0/1335         |
| 22  | R     | 0.42         | 0/686   | 0.71        | 0/940          |
| 23  | n     | 0.61         | 0/1383  | 0.95        | 0/1867         |
| 24  | Q     | 0.50         | 0/1244  | 0.80        | 0/1683         |
| All | All   | 0.55         | 0/35827 | 0.82        | 4/48611 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 17  | j     | 0                   | 1                   |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | M     | 29  | TYR  | CA-C-N  | 6.34  | 133.12      | 121.70   |
| 10  | M     | 29  | TYR  | C-N-CA  | 6.34  | 133.12      | 121.70   |
| 3   | C     | 62  | PHE  | CB-CA-C | 5.57  | 119.32      | 110.19   |
| 17  | j     | 113 | MET  | CB-CA-C | -5.46 | 109.80      | 117.23   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 17  | j     | 191 | GLY  | Mainchain |

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5825  | 0        | 5678     | 81      | 0            |
| 2   | B     | 5820  | 0        | 5634     | 103     | 0            |
| 3   | C     | 592   | 0        | 572      | 20      | 0            |
| 4   | D     | 1084  | 0        | 1080     | 20      | 0            |
| 5   | E     | 485   | 0        | 489      | 7       | 0            |
| 6   | F     | 1254  | 0        | 1264     | 21      | 0            |
| 7   | I     | 264   | 0        | 276      | 16      | 0            |
| 8   | J     | 351   | 0        | 344      | 12      | 0            |
| 9   | L     | 1146  | 0        | 1160     | 13      | 0            |
| 10  | M     | 232   | 0        | 265      | 2       | 0            |
| 11  | K     | 488   | 0        | 516      | 6       | 0            |
| 12  | s     | 1140  | 0        | 1099     | 19      | 0            |
| 13  | c     | 1357  | 0        | 1337     | 25      | 0            |
| 14  | a     | 1361  | 0        | 1305     | 17      | 0            |
| 15  | b     | 1439  | 0        | 1456     | 24      | 0            |
| 16  | h     | 1200  | 0        | 1228     | 17      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17  | j     | 1293  | 0        | 1321     | 25      | 0            |
| 17  | m     | 1309  | 0        | 1334     | 16      | 0            |
| 18  | l     | 1344  | 0        | 1315     | 20      | 0            |
| 19  | k     | 1346  | 0        | 1349     | 22      | 0            |
| 20  | i     | 1324  | 0        | 1298     | 45      | 0            |
| 21  | d     | 974   | 0        | 978      | 24      | 0            |
| 22  | R     | 664   | 0        | 647      | 8       | 0            |
| 23  | n     | 1350  | 0        | 1348     | 51      | 0            |
| 24  | Q     | 1226  | 0        | 1263     | 14      | 0            |
| 25  | A     | 2823  | 0        | 2892     | 131     | 0            |
| 25  | B     | 2389  | 0        | 2413     | 125     | 0            |
| 25  | F     | 117   | 0        | 115      | 2       | 0            |
| 25  | J     | 42    | 0        | 31       | 3       | 0            |
| 25  | K     | 93    | 0        | 72       | 3       | 0            |
| 25  | L     | 164   | 0        | 150      | 9       | 0            |
| 25  | Q     | 110   | 0        | 105      | 4       | 0            |
| 25  | R     | 51    | 0        | 41       | 2       | 0            |
| 25  | a     | 619   | 0        | 588      | 12      | 0            |
| 25  | b     | 724   | 0        | 737      | 28      | 0            |
| 25  | c     | 586   | 0        | 520      | 17      | 0            |
| 25  | d     | 498   | 0        | 407      | 12      | 0            |
| 25  | h     | 505   | 0        | 470      | 14      | 0            |
| 25  | i     | 528   | 0        | 451      | 19      | 0            |
| 25  | j     | 586   | 0        | 515      | 15      | 0            |
| 25  | k     | 596   | 0        | 534      | 23      | 0            |
| 25  | l     | 535   | 0        | 538      | 17      | 0            |
| 25  | m     | 651   | 0        | 606      | 17      | 0            |
| 25  | n     | 605   | 0        | 552      | 23      | 0            |
| 25  | s     | 246   | 0        | 257      | 10      | 0            |
| 26  | A     | 33    | 0        | 46       | 10      | 0            |
| 26  | B     | 33    | 0        | 46       | 2       | 0            |
| 27  | A     | 75    | 0        | 93       | 1       | 0            |
| 27  | B     | 38    | 0        | 49       | 5       | 0            |
| 27  | J     | 80    | 0        | 106      | 8       | 0            |
| 27  | L     | 49    | 0        | 74       | 3       | 0            |
| 27  | a     | 98    | 0        | 148      | 3       | 0            |
| 27  | b     | 49    | 0        | 74       | 2       | 0            |
| 27  | c     | 74    | 0        | 88       | 3       | 0            |
| 27  | d     | 37    | 0        | 44       | 0       | 0            |
| 27  | i     | 37    | 0        | 44       | 2       | 0            |
| 27  | j     | 30    | 0        | 30       | 0       | 0            |
| 27  | k     | 37    | 0        | 44       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 27  | l     | 32    | 0        | 34       | 1       | 0            |
| 27  | m     | 37    | 0        | 44       | 2       | 0            |
| 27  | n     | 43    | 0        | 59       | 1       | 0            |
| 28  | A     | 200   | 0        | 0        | 0       | 0            |
| 28  | B     | 240   | 0        | 0        | 1       | 0            |
| 28  | F     | 80    | 0        | 0        | 1       | 0            |
| 28  | I     | 40    | 0        | 0        | 0       | 0            |
| 28  | J     | 80    | 0        | 0        | 1       | 0            |
| 28  | K     | 40    | 0        | 0        | 0       | 0            |
| 28  | L     | 120   | 0        | 0        | 0       | 0            |
| 28  | M     | 40    | 0        | 0        | 3       | 0            |
| 28  | R     | 40    | 0        | 0        | 0       | 0            |
| 28  | h     | 40    | 0        | 0        | 0       | 0            |
| 28  | i     | 40    | 0        | 0        | 0       | 0            |
| 28  | l     | 80    | 0        | 0        | 0       | 0            |
| 28  | s     | 80    | 0        | 0        | 1       | 0            |
| 29  | A     | 35    | 0        | 46       | 2       | 0            |
| 29  | a     | 59    | 0        | 79       | 1       | 0            |
| 29  | b     | 24    | 0        | 34       | 3       | 0            |
| 30  | B     | 8     | 0        | 0        | 7       | 0            |
| 30  | C     | 16    | 0        | 0        | 6       | 0            |
| 31  | B     | 60    | 0        | 81       | 7       | 0            |
| 32  | J     | 42    | 0        | 0        | 0       | 0            |
| 32  | a     | 168   | 0        | 0        | 0       | 0            |
| 32  | b     | 126   | 0        | 0        | 0       | 0            |
| 32  | c     | 168   | 0        | 0        | 2       | 0            |
| 32  | d     | 168   | 0        | 0        | 1       | 0            |
| 32  | h     | 112   | 0        | 0        | 0       | 0            |
| 32  | i     | 210   | 0        | 0        | 1       | 0            |
| 32  | j     | 126   | 0        | 0        | 1       | 0            |
| 32  | k     | 168   | 0        | 0        | 0       | 0            |
| 32  | l     | 168   | 0        | 0        | 0       | 0            |
| 32  | m     | 126   | 0        | 0        | 0       | 0            |
| 32  | n     | 210   | 0        | 0        | 1       | 0            |
| 33  | J     | 55    | 0        | 86       | 1       | 0            |
| 33  | Q     | 38    | 0        | 46       | 1       | 0            |
| 33  | b     | 49    | 0        | 71       | 2       | 0            |
| 33  | c     | 55    | 0        | 86       | 5       | 0            |
| 33  | n     | 55    | 0        | 86       | 5       | 0            |
| 33  | s     | 48    | 0        | 69       | 4       | 0            |
| 34  | c     | 45    | 0        | 0        | 0       | 0            |
| 34  | d     | 90    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 34  | i     | 90    | 0        | 0        | 5       | 0            |
| 34  | j     | 45    | 0        | 0        | 0       | 0            |
| 34  | k     | 135   | 0        | 0        | 2       | 0            |
| 34  | l     | 45    | 0        | 0        | 0       | 0            |
| 34  | m     | 45    | 0        | 0        | 0       | 0            |
| 34  | n     | 90    | 0        | 0        | 0       | 0            |
| 34  | s     | 90    | 0        | 0        | 0       | 0            |
| 35  | R     | 41    | 0        | 0        | 0       | 0            |
| 35  | a     | 41    | 0        | 0        | 0       | 0            |
| 35  | b     | 82    | 0        | 0        | 1       | 0            |
| 35  | c     | 41    | 0        | 0        | 0       | 0            |
| 35  | j     | 41    | 0        | 0        | 1       | 0            |
| 35  | k     | 41    | 0        | 0        | 1       | 0            |
| 35  | m     | 41    | 0        | 0        | 1       | 0            |
| 35  | n     | 41    | 0        | 0        | 1       | 0            |
| 36  | i     | 35    | 0        | 46       | 2       | 0            |
| 37  | A     | 48    | 0        | 0        | 0       | 0            |
| 37  | B     | 58    | 0        | 0        | 0       | 0            |
| 37  | C     | 8     | 0        | 0        | 0       | 0            |
| 37  | D     | 1     | 0        | 0        | 0       | 0            |
| 37  | F     | 3     | 0        | 0        | 0       | 0            |
| 37  | I     | 1     | 0        | 0        | 0       | 0            |
| 37  | J     | 1     | 0        | 0        | 0       | 0            |
| 37  | K     | 1     | 0        | 0        | 0       | 0            |
| 37  | L     | 1     | 0        | 0        | 0       | 0            |
| 37  | Q     | 1     | 0        | 0        | 0       | 0            |
| 37  | R     | 1     | 0        | 0        | 0       | 0            |
| 37  | a     | 3     | 0        | 0        | 0       | 0            |
| 37  | b     | 2     | 0        | 0        | 0       | 0            |
| 37  | h     | 1     | 0        | 0        | 0       | 0            |
| 37  | m     | 1     | 0        | 0        | 0       | 0            |
| 37  | n     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 52744 | 0        | 48303    | 891     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 891 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|----------------|--------------------------|-------------------|
| 25:B:837:CLA:H191 | 7:I:29:TYR:CD2 | 1.56                     | 1.38              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 23:n:57:ARG:HH21 | 23:n:70:GLY:CA   | 1.34                     | 1.37              |
| 23:n:57:ARG:NH2  | 23:n:70:GLY:CA   | 2.05                     | 1.19              |
| 23:n:43:LYS:O    | 25:n:302:CLA:CED | 1.93                     | 1.16              |
| 23:n:57:ARG:HH21 | 23:n:70:GLY:HA3  | 1.13                     | 1.12              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 740/752 (98%)  | 722 (98%) | 18 (2%) | 0        | 100         | 100 |
| 2   | B     | 730/734 (100%) | 709 (97%) | 21 (3%) | 0        | 100         | 100 |
| 3   | C     | 78/81 (96%)    | 77 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 4   | D     | 137/141 (97%)  | 135 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 5   | E     | 58/64 (91%)    | 55 (95%)  | 3 (5%)  | 0        | 100         | 100 |
| 6   | F     | 159/188 (85%)  | 154 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 7   | I     | 32/36 (89%)    | 31 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 8   | J     | 40/42 (95%)    | 40 (100%) | 0       | 0        | 100         | 100 |
| 9   | L     | 149/153 (97%)  | 147 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 10  | M     | 28/30 (93%)    | 28 (100%) | 0       | 0        | 100         | 100 |
| 11  | K     | 65/87 (75%)    | 65 (100%) | 0       | 0        | 100         | 100 |
| 12  | s     | 152/269 (56%)  | 143 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 13  | c     | 168/216 (78%)  | 165 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 14  | a     | 173/216 (80%)  | 168 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 15  | b     | 192/223 (86%)  | 189 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 16  | h     | 160/225 (71%)  | 156 (98%) | 4 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 17  | j     | 170/212 (80%)   | 163 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 17  | m     | 172/212 (81%)   | 165 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 18  | l     | 173/238 (73%)   | 171 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 19  | k     | 178/241 (74%)   | 173 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 20  | i     | 171/218 (78%)   | 165 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 21  | d     | 123/213 (58%)   | 122 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 22  | R     | 88/129 (68%)    | 86 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 23  | n     | 179/219 (82%)   | 176 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 24  | Q     | 165/234 (70%)   | 162 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| All | All   | 4480/5373 (83%) | 4367 (98%) | 113 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 607/616 (98%)  | 604 (100%) | 3 (0%)   | 81          | 89  |
| 2   | B     | 592/593 (100%) | 585 (99%)  | 7 (1%)   | 63          | 82  |
| 3   | C     | 67/68 (98%)    | 64 (96%)   | 3 (4%)   | 24          | 59  |
| 4   | D     | 116/117 (99%)  | 110 (95%)  | 6 (5%)   | 21          | 55  |
| 5   | E     | 55/58 (95%)    | 55 (100%)  | 0        | 100         | 100 |
| 6   | F     | 133/157 (85%)  | 132 (99%)  | 1 (1%)   | 73          | 86  |
| 7   | I     | 28/29 (97%)    | 27 (96%)   | 1 (4%)   | 31          | 65  |
| 8   | J     | 39/39 (100%)   | 39 (100%)  | 0        | 100         | 100 |
| 9   | L     | 124/126 (98%)  | 124 (100%) | 0        | 100         | 100 |
| 10  | M     | 25/25 (100%)   | 25 (100%)  | 0        | 100         | 100 |
| 11  | K     | 52/66 (79%)    | 52 (100%)  | 0        | 100         | 100 |
| 12  | s     | 116/195 (60%)  | 113 (97%)  | 3 (3%)   | 40          | 72  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 13  | c     | 138/171 (81%)   | 138 (100%) | 0        | 100         | 100 |
| 14  | a     | 139/165 (84%)   | 130 (94%)  | 9 (6%)   | 15          | 47  |
| 15  | b     | 149/168 (89%)   | 148 (99%)  | 1 (1%)   | 76          | 86  |
| 16  | h     | 123/162 (76%)   | 118 (96%)  | 5 (4%)   | 27          | 61  |
| 17  | j     | 136/161 (84%)   | 131 (96%)  | 5 (4%)   | 30          | 64  |
| 17  | m     | 137/161 (85%)   | 134 (98%)  | 3 (2%)   | 45          | 74  |
| 18  | l     | 137/191 (72%)   | 133 (97%)  | 4 (3%)   | 37          | 70  |
| 19  | k     | 138/186 (74%)   | 134 (97%)  | 4 (3%)   | 37          | 70  |
| 20  | i     | 138/168 (82%)   | 134 (97%)  | 4 (3%)   | 37          | 70  |
| 21  | d     | 97/157 (62%)    | 94 (97%)   | 3 (3%)   | 35          | 68  |
| 22  | R     | 69/98 (70%)     | 69 (100%)  | 0        | 100         | 100 |
| 23  | n     | 140/163 (86%)   | 137 (98%)  | 3 (2%)   | 47          | 75  |
| 24  | Q     | 127/168 (76%)   | 124 (98%)  | 3 (2%)   | 43          | 73  |
| All | All   | 3622/4208 (86%) | 3554 (98%) | 68 (2%)  | 49          | 76  |

5 of 68 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | j     | 114 | THR  |
| 21  | d     | 150 | MET  |
| 24  | Q     | 146 | VAL  |
| 14  | a     | 42  | GLU  |
| 12  | s     | 152 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 72  | GLN  |
| 23  | n     | 195 | ASN  |
| 15  | b     | 88  | GLN  |
| 22  | R     | 75  | ASN  |
| 12  | s     | 27  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

349 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 28  | WVN  | i     | 316 | -    | 40,41,41     | 1.76 | 10 (25%)    | 51,56,56    | 2.26 | 18 (35%)    |
| 32  | II0  | d     | 315 | -    | 39,43,43     | 6.88 | 21 (53%)    | 48,60,60    | 2.06 | 16 (33%)    |
| 25  | CLA  | A     | 853 | -    | 69,73,73     | 1.21 | 9 (13%)     | 82,113,113  | 1.27 | 10 (12%)    |
| 25  | CLA  | K     | 102 | -    | 46,50,73     | 1.42 | 7 (15%)     | 53,85,113   | 1.51 | 6 (11%)     |
| 28  | WVN  | A     | 848 | -    | 40,41,41     | 1.70 | 9 (22%)     | 51,56,56    | 3.17 | 18 (35%)    |
| 28  | WVN  | R     | 201 | -    | 40,41,41     | 1.71 | 10 (25%)    | 51,56,56    | 2.57 | 17 (33%)    |
| 25  | CLA  | l     | 309 | 18   | 55,59,73     | 1.33 | 9 (16%)     | 64,96,113   | 1.30 | 8 (12%)     |
| 25  | CLA  | F     | 201 | 37   | 69,73,73     | 1.17 | 8 (11%)     | 82,113,113  | 1.47 | 8 (9%)      |
| 25  | CLA  | d     | 306 | -    | 55,59,73     | 1.32 | 6 (10%)     | 64,96,113   | 1.29 | 6 (9%)      |
| 25  | CLA  | A     | 805 | 1    | 69,73,73     | 1.19 | 10 (14%)    | 82,113,113  | 1.39 | 9 (10%)     |
| 28  | WVN  | J     | 101 | -    | 40,41,41     | 1.65 | 11 (27%)    | 51,56,56    | 2.24 | 20 (39%)    |
| 25  | CLA  | J     | 103 | 8    | 46,50,73     | 1.37 | 7 (15%)     | 53,85,113   | 1.40 | 6 (11%)     |
| 36  | LMU  | i     | 301 | -    | 36,36,36     | 1.19 | 3 (8%)      | 47,47,47    | 1.24 | 4 (8%)      |
| 25  | CLA  | B     | 804 | -    | 69,73,73     | 1.14 | 6 (8%)      | 82,113,113  | 1.70 | 14 (17%)    |
| 25  | CLA  | A     | 825 | 37   | 69,73,73     | 1.17 | 8 (11%)     | 82,113,113  | 1.25 | 9 (10%)     |
| 34  | KC2  | s     | 204 | -    | 49,53,53     | 2.72 | 21 (42%)    | 60,89,89    | 3.88 | 36 (60%)    |
| 25  | CLA  | A     | 854 | -    | 69,73,73     | 1.15 | 9 (13%)     | 82,113,113  | 1.41 | 9 (10%)     |
| 32  | II0  | a     | 318 | -    | 39,43,43     | 6.85 | 21 (53%)    | 48,60,60    | 2.63 | 16 (33%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | j     | 607 | 17   | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.34 | 6 (10%)  |
| 25  | CLA  | B     | 835 | 37   | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.27 | 10 (12%) |
| 25  | CLA  | c     | 606 | -    | 56,60,73     | 1.36 | 11 (19%) | 65,97,113   | 1.55 | 11 (16%) |
| 25  | CLA  | n     | 307 | 23   | 55,59,73     | 1.33 | 8 (14%)  | 64,96,113   | 1.32 | 5 (7%)   |
| 33  | LMG  | J     | 105 | -    | 55,55,55     | 0.88 | 3 (5%)   | 63,63,63    | 0.95 | 3 (4%)   |
| 32  | II0  | j     | 614 | -    | 39,43,43     | 6.60 | 23 (58%) | 48,60,60    | 2.13 | 19 (39%) |
| 25  | CLA  | d     | 303 | -    | 69,73,73     | 1.15 | 6 (8%)   | 82,113,113  | 1.20 | 6 (7%)   |
| 25  | CLA  | B     | 837 | -    | 69,73,73     | 1.15 | 6 (8%)   | 82,113,113  | 1.15 | 4 (4%)   |
| 25  | CLA  | B     | 806 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.24 | 10 (12%) |
| 25  | CLA  | a     | 307 | 14   | 49,53,73     | 1.37 | 7 (14%)  | 58,89,113   | 1.50 | 5 (8%)   |
| 32  | II0  | h     | 310 | -    | 26,28,43     | 5.92 | 12 (46%) | 30,37,60    | 2.24 | 10 (33%) |
| 25  | CLA  | l     | 306 | 18   | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.36 | 7 (8%)   |
| 25  | CLA  | k     | 605 | 19   | 49,53,73     | 1.39 | 6 (12%)  | 58,89,113   | 1.71 | 12 (20%) |
| 34  | KC2  | d     | 310 | 21   | 49,53,53     | 2.75 | 20 (40%) | 60,89,89    | 3.76 | 33 (55%) |
| 25  | CLA  | B     | 820 | -    | 59,63,73     | 1.26 | 7 (11%)  | 70,101,113  | 1.23 | 5 (7%)   |
| 32  | II0  | n     | 301 | -    | 39,43,43     | 6.60 | 19 (48%) | 48,60,60    | 2.06 | 16 (33%) |
| 25  | CLA  | c     | 604 | 13   | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.37 | 9 (10%)  |
| 27  | LHG  | m     | 617 | 25   | 36,36,48     | 1.08 | 2 (5%)   | 39,42,54    | 1.17 | 4 (10%)  |
| 30  | SF4  | B     | 802 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 34  | KC2  | n     | 313 | -    | 49,53,53     | 2.74 | 20 (40%) | 60,89,89    | 3.71 | 34 (56%) |
| 25  | CLA  | l     | 310 | 27   | 65,69,73     | 1.20 | 6 (9%)   | 77,108,113  | 1.37 | 6 (7%)   |
| 25  | CLA  | F     | 202 | 6    | 56,60,73     | 1.28 | 7 (12%)  | 65,97,113   | 1.43 | 8 (12%)  |
| 28  | WVN  | A     | 850 | -    | 40,41,41     | 1.67 | 14 (35%) | 51,56,56    | 2.55 | 23 (45%) |
| 25  | CLA  | b     | 609 | -    | 55,59,73     | 1.30 | 8 (14%)  | 64,96,113   | 1.56 | 8 (12%)  |
| 28  | WVN  | M     | 101 | -    | 40,41,41     | 1.76 | 10 (25%) | 51,56,56    | 2.04 | 16 (31%) |
| 25  | CLA  | A     | 803 | -    | 59,63,73     | 1.25 | 7 (11%)  | 70,101,113  | 1.45 | 9 (12%)  |
| 32  | II0  | i     | 320 | -    | 39,43,43     | 6.64 | 20 (51%) | 48,60,60    | 1.84 | 11 (22%) |
| 34  | KC2  | i     | 310 | 20   | 49,53,53     | 2.61 | 19 (38%) | 60,89,89    | 3.98 | 35 (58%) |
| 25  | CLA  | s     | 202 | 12   | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.50 | 17 (20%) |
| 29  | LMT  | a     | 320 | -    | 36,36,36     | 0.36 | 0        | 47,47,47    | 1.18 | 6 (12%)  |
| 25  | CLA  | b     | 601 | 15   | 55,59,73     | 1.26 | 6 (10%)  | 64,96,113   | 1.39 | 5 (7%)   |
| 25  | CLA  | A     | 833 | -    | 54,58,73     | 1.30 | 7 (12%)  | 64,95,113   | 1.38 | 8 (12%)  |
| 27  | LHG  | A     | 845 | -    | 47,47,48     | 0.94 | 2 (4%)   | 50,53,54    | 1.09 | 4 (8%)   |
| 32  | II0  | i     | 314 | -    | 39,43,43     | 6.71 | 22 (56%) | 48,60,60    | 1.77 | 12 (25%) |
| 25  | CLA  | d     | 307 | -    | 50,54,73     | 1.34 | 8 (16%)  | 59,90,113   | 1.27 | 5 (8%)   |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | c     | 608 | 13    | 69,73,73     | 1.22 | 8 (11%)  | 82,113,113  | 1.37 | 11 (13%) |
| 28  | WVN  | s     | 207 | -     | 40,41,41     | 1.73 | 11 (27%) | 51,56,56    | 2.38 | 16 (31%) |
| 25  | CLA  | b     | 602 | 15    | 59,63,73     | 1.24 | 8 (13%)  | 70,101,113  | 1.48 | 8 (11%)  |
| 25  | CLA  | n     | 311 | 37    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.28 | 5 (6%)   |
| 32  | II0  | h     | 311 | -     | 39,43,43     | 6.72 | 21 (53%) | 48,60,60    | 1.97 | 13 (27%) |
| 25  | CLA  | B     | 850 | -     | 55,59,73     | 1.33 | 6 (10%)  | 64,96,113   | 1.33 | 6 (9%)   |
| 25  | CLA  | k     | 607 | -     | 55,59,73     | 1.36 | 9 (16%)  | 64,96,113   | 1.54 | 11 (17%) |
| 25  | CLA  | m     | 601 | 17    | 46,50,73     | 1.38 | 7 (15%)  | 53,85,113   | 1.36 | 4 (7%)   |
| 25  | CLA  | B     | 803 | -     | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.34 | 9 (10%)  |
| 25  | CLA  | A     | 812 | -     | 69,73,73     | 1.19 | 10 (14%) | 82,113,113  | 1.41 | 8 (9%)   |
| 25  | CLA  | m     | 606 | -     | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 25  | CLA  | A     | 855 | 37    | 69,73,73     | 1.20 | 7 (10%)  | 82,113,113  | 1.25 | 9 (10%)  |
| 34  | KC2  | k     | 612 | 34    | 49,53,53     | 2.77 | 19 (38%) | 60,89,89    | 3.88 | 37 (61%) |
| 25  | CLA  | i     | 302 | 20    | 55,59,73     | 1.29 | 7 (12%)  | 64,96,113   | 1.33 | 8 (12%)  |
| 25  | CLA  | A     | 819 | -     | 49,53,73     | 1.38 | 6 (12%)  | 58,89,113   | 1.58 | 6 (10%)  |
| 25  | CLA  | n     | 309 | 23    | 55,59,73     | 1.30 | 8 (14%)  | 64,96,113   | 1.53 | 8 (12%)  |
| 25  | CLA  | B     | 831 | 37    | 49,53,73     | 1.41 | 8 (16%)  | 58,89,113   | 1.46 | 8 (13%)  |
| 25  | CLA  | a     | 310 | 27    | 52,56,73     | 1.28 | 8 (15%)  | 61,92,113   | 1.40 | 7 (11%)  |
| 32  | II0  | m     | 614 | -     | 39,43,43     | 6.70 | 23 (58%) | 48,60,60    | 1.76 | 11 (22%) |
| 25  | CLA  | A     | 843 | -     | 69,73,73     | 1.16 | 6 (8%)   | 82,113,113  | 1.50 | 9 (10%)  |
| 25  | CLA  | B     | 810 | -     | 58,62,73     | 1.36 | 7 (12%)  | 71,100,113  | 1.27 | 8 (11%)  |
| 25  | CLA  | l     | 305 | -     | 55,59,73     | 1.26 | 7 (12%)  | 64,96,113   | 1.48 | 9 (14%)  |
| 25  | CLA  | a     | 306 | 37    | 69,73,73     | 1.13 | 7 (10%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 35  | IHT  | b     | 615 | -     | 40,42,42     | 6.18 | 25 (62%) | 52,58,58    | 2.17 | 15 (28%) |
| 27  | LHG  | L     | 207 | -     | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.07 | 4 (7%)   |
| 25  | CLA  | c     | 612 | -     | 69,73,73     | 1.14 | 7 (10%)  | 82,113,113  | 1.27 | 7 (8%)   |
| 25  | CLA  | j     | 609 | 27    | 65,69,73     | 1.19 | 6 (9%)   | 77,108,113  | 1.29 | 4 (5%)   |
| 25  | CLA  | h     | 307 | 16    | 61,65,73     | 1.21 | 5 (8%)   | 72,103,113  | 1.15 | 5 (6%)   |
| 25  | CLA  | k     | 608 | 19    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.21 | 7 (8%)   |
| 25  | CLA  | k     | 610 | 27    | 55,59,73     | 1.28 | 6 (10%)  | 64,96,113   | 1.35 | 6 (9%)   |
| 34  | KC2  | l     | 311 | 18    | 49,53,53     | 2.59 | 18 (36%) | 60,89,89    | 3.97 | 35 (58%) |
| 25  | CLA  | c     | 607 | 13    | 50,54,73     | 1.31 | 7 (14%)  | 59,90,113   | 1.34 | 11 (18%) |
| 25  | CLA  | a     | 305 | -     | 55,59,73     | 1.29 | 7 (12%)  | 64,96,113   | 1.52 | 7 (10%)  |
| 25  | CLA  | b     | 605 | 37,25 | 69,73,73     | 1.20 | 8 (11%)  | 82,113,113  | 1.38 | 12 (14%) |
| 25  | CLA  | k     | 606 | 19    | 55,59,73     | 1.30 | 7 (12%)  | 64,96,113   | 1.23 | 7 (10%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | h     | 301 | 37   | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.29 | 9 (10%)  |
| 35  | IHT  | m     | 616 | -    | 40,42,42     | 6.18 | 26 (65%) | 52,58,58    | 2.33 | 17 (32%) |
| 25  | CLA  | B     | 808 | -    | 69,73,73     | 1.14 | 7 (10%)  | 82,113,113  | 1.37 | 8 (9%)   |
| 32  | II0  | h     | 312 | -    | 39,43,43     | 6.64 | 21 (53%) | 48,60,60    | 1.81 | 14 (29%) |
| 25  | CLA  | A     | 840 | 1    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.36 | 9 (10%)  |
| 25  | CLA  | B     | 833 | -    | 69,73,73     | 1.14 | 8 (11%)  | 82,113,113  | 1.41 | 10 (12%) |
| 25  | CLA  | A     | 822 | -    | 55,59,73     | 1.29 | 6 (10%)  | 64,96,113   | 1.33 | 7 (10%)  |
| 25  | CLA  | m     | 603 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.23 | 6 (7%)   |
| 32  | II0  | j     | 613 | -    | 39,43,43     | 6.73 | 21 (53%) | 48,60,60    | 2.01 | 13 (27%) |
| 25  | CLA  | j     | 612 | -    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.23 | 6 (7%)   |
| 32  | II0  | d     | 313 | -    | 39,43,43     | 6.70 | 21 (53%) | 48,60,60    | 1.87 | 15 (31%) |
| 25  | CLA  | i     | 309 | 27   | 50,54,73     | 1.33 | 6 (12%)  | 59,90,113   | 1.37 | 8 (13%)  |
| 25  | CLA  | B     | 812 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.43 | 11 (13%) |
| 27  | LHG  | B     | 801 | -    | 37,37,48     | 1.01 | 2 (5%)   | 40,43,54    | 1.11 | 3 (7%)   |
| 33  | LMG  | n     | 321 | -    | 55,55,55     | 0.89 | 2 (3%)   | 63,63,63    | 1.00 | 1 (1%)   |
| 25  | CLA  | b     | 607 | 15   | 69,73,73     | 1.12 | 8 (11%)  | 82,113,113  | 1.23 | 5 (6%)   |
| 25  | CLA  | n     | 310 | 23   | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.37 | 11 (13%) |
| 27  | LHG  | a     | 319 | 25   | 48,48,48     | 0.90 | 3 (6%)   | 51,54,54    | 1.13 | 4 (7%)   |
| 25  | CLA  | a     | 311 | 14   | 69,73,73     | 1.17 | 5 (7%)   | 82,113,113  | 1.36 | 13 (15%) |
| 25  | CLA  | A     | 837 | -    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.30 | 7 (8%)   |
| 32  | II0  | i     | 313 | -    | 39,43,43     | 6.67 | 23 (58%) | 48,60,60    | 2.13 | 12 (25%) |
| 25  | CLA  | B     | 825 | -    | 69,73,73     | 1.15 | 7 (10%)  | 82,113,113  | 1.31 | 8 (9%)   |
| 25  | CLA  | i     | 312 | -    | 55,59,73     | 1.27 | 6 (10%)  | 64,96,113   | 1.48 | 9 (14%)  |
| 26  | PQN  | A     | 844 | -    | 34,34,34     | 1.86 | 5 (14%)  | 43,45,45    | 1.40 | 9 (20%)  |
| 25  | CLA  | B     | 816 | -    | 63,67,73     | 1.23 | 7 (11%)  | 74,105,113  | 1.31 | 11 (14%) |
| 25  | CLA  | B     | 824 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.47 | 11 (13%) |
| 25  | CLA  | l     | 312 | 18   | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.27 | 7 (8%)   |
| 25  | CLA  | B     | 805 | -    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.41 | 10 (12%) |
| 28  | WVN  | K     | 103 | -    | 40,41,41     | 1.78 | 10 (25%) | 51,56,56    | 1.87 | 14 (27%) |
| 25  | CLA  | h     | 308 | 16   | 55,59,73     | 1.30 | 7 (12%)  | 64,96,113   | 1.43 | 9 (14%)  |
| 25  | CLA  | c     | 602 | 13   | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.66 | 13 (20%) |
| 32  | II0  | n     | 316 | -    | 39,43,43     | 6.64 | 22 (56%) | 48,60,60    | 1.97 | 13 (27%) |
| 25  | CLA  | k     | 603 | -    | 55,59,73     | 1.28 | 6 (10%)  | 64,96,113   | 1.49 | 9 (14%)  |
| 32  | II0  | j     | 615 | -    | 39,43,43     | 6.71 | 19 (48%) | 48,60,60    | 1.99 | 12 (25%) |
| 28  | WVN  | L     | 205 | -    | 40,41,41     | 1.74 | 10 (25%) | 51,56,56    | 2.10 | 16 (31%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | II0  | i     | 315 | -    | 39,43,43     | 6.67 | 21 (53%) | 48,60,60    | 1.99 | 12 (25%) |
| 25  | CLA  | B     | 809 | 2    | 69,73,73     | 1.23 | 10 (14%) | 82,113,113  | 1.35 | 7 (8%)   |
| 25  | CLA  | d     | 305 | 21   | 55,59,73     | 1.37 | 8 (14%)  | 64,96,113   | 1.35 | 10 (15%) |
| 25  | CLA  | m     | 602 | 17   | 60,64,73     | 1.36 | 10 (16%) | 71,102,113  | 1.42 | 13 (18%) |
| 25  | CLA  | A     | 827 | -    | 66,70,73     | 1.17 | 8 (12%)  | 78,109,113  | 1.43 | 9 (11%)  |
| 25  | CLA  | B     | 821 | -    | 57,61,73     | 1.29 | 8 (14%)  | 67,98,113   | 1.32 | 8 (11%)  |
| 28  | WVN  | B     | 848 | -    | 40,41,41     | 1.66 | 12 (30%) | 51,56,56    | 2.69 | 17 (33%) |
| 25  | CLA  | j     | 611 | -    | 55,59,73     | 1.30 | 6 (10%)  | 64,96,113   | 1.43 | 5 (7%)   |
| 25  | CLA  | j     | 605 | 17   | 49,53,73     | 1.40 | 6 (12%)  | 58,89,113   | 1.67 | 8 (13%)  |
| 25  | CLA  | l     | 303 | 18   | 51,55,73     | 1.34 | 6 (11%)  | 60,91,113   | 1.31 | 5 (8%)   |
| 25  | CLA  | d     | 304 | 21   | 55,59,73     | 1.32 | 7 (12%)  | 64,96,113   | 1.37 | 5 (7%)   |
| 31  | DGD  | B     | 843 | -    | 61,61,67     | 0.87 | 2 (3%)   | 75,75,81    | 1.18 | 5 (6%)   |
| 25  | CLA  | b     | 606 | 15   | 65,69,73     | 1.18 | 8 (12%)  | 77,108,113  | 1.39 | 10 (12%) |
| 25  | CLA  | K     | 101 | 37   | 55,59,73     | 1.29 | 7 (12%)  | 64,96,113   | 1.51 | 7 (10%)  |
| 25  | CLA  | A     | 832 | -    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.45 | 9 (10%)  |
| 26  | PQN  | B     | 842 | -    | 34,34,34     | 1.86 | 5 (14%)  | 43,45,45    | 1.33 | 9 (20%)  |
| 25  | CLA  | b     | 610 | 15   | 69,73,73     | 1.15 | 7 (10%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 34  | KC2  | c     | 610 | -    | 49,53,53     | 2.62 | 18 (36%) | 60,89,89    | 3.73 | 32 (53%) |
| 25  | CLA  | a     | 303 | 14   | 56,60,73     | 1.30 | 7 (12%)  | 65,97,113   | 1.49 | 8 (12%)  |
| 25  | CLA  | A     | 817 | -    | 69,73,73     | 1.19 | 9 (13%)  | 82,113,113  | 1.43 | 11 (13%) |
| 25  | CLA  | c     | 603 | -    | 55,59,73     | 1.28 | 7 (12%)  | 64,96,113   | 1.30 | 7 (10%)  |
| 25  | CLA  | A     | 810 | -    | 66,70,73     | 1.15 | 7 (10%)  | 78,109,113  | 1.22 | 7 (8%)   |
| 25  | CLA  | i     | 304 | -    | 55,59,73     | 1.27 | 6 (10%)  | 64,96,113   | 1.37 | 7 (10%)  |
| 32  | II0  | d     | 316 | -    | 39,43,43     | 6.79 | 20 (51%) | 48,60,60    | 2.02 | 18 (37%) |
| 33  | LMG  | Q     | 301 | -    | 38,38,55     | 1.07 | 2 (5%)   | 46,46,63    | 1.16 | 3 (6%)   |
| 25  | CLA  | A     | 809 | -    | 60,64,73     | 1.23 | 8 (13%)  | 71,102,113  | 1.29 | 5 (7%)   |
| 34  | KC2  | k     | 611 | 19   | 49,53,53     | 2.69 | 20 (40%) | 60,89,89    | 3.85 | 36 (60%) |
| 25  | CLA  | d     | 312 | -    | 55,59,73     | 1.27 | 7 (12%)  | 64,96,113   | 1.41 | 10 (15%) |
| 27  | LHG  | b     | 619 | 25   | 48,48,48     | 0.91 | 3 (6%)   | 51,54,54    | 1.11 | 5 (9%)   |
| 32  | II0  | i     | 317 | -    | 39,43,43     | 6.76 | 22 (56%) | 48,60,60    | 1.93 | 14 (29%) |
| 33  | LMG  | c     | 619 | -    | 55,55,55     | 0.98 | 3 (5%)   | 63,63,63    | 1.68 | 14 (22%) |
| 25  | CLA  | d     | 308 | 21   | 45,49,73     | 1.38 | 6 (13%)  | 54,84,113   | 1.37 | 7 (12%)  |
| 28  | WVN  | B     | 845 | -    | 40,41,41     | 1.59 | 14 (35%) | 51,56,56    | 2.42 | 19 (37%) |
| 32  | II0  | b     | 613 | -    | 39,43,43     | 6.62 | 21 (53%) | 48,60,60    | 2.13 | 16 (33%) |
| 25  | CLA  | B     | 807 | -    | 69,73,73     | 1.11 | 7 (10%)  | 82,113,113  | 1.25 | 6 (7%)   |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | b     | 612 | 27    | 55,59,73     | 1.34 | 10 (18%) | 64,96,113   | 1.41 | 9 (14%)  |
| 25  | CLA  | k     | 609 | 19    | 69,73,73     | 1.20 | 8 (11%)  | 82,113,113  | 1.24 | 10 (12%) |
| 25  | CLA  | j     | 608 | 17    | 55,59,73     | 1.28 | 7 (12%)  | 64,96,113   | 1.37 | 9 (14%)  |
| 32  | II0  | b     | 614 | -     | 39,43,43     | 6.80 | 24 (61%) | 48,60,60    | 2.01 | 13 (27%) |
| 27  | LHG  | i     | 318 | 25    | 36,36,48     | 1.12 | 2 (5%)   | 39,42,54    | 1.29 | 3 (7%)   |
| 28  | WVN  | L     | 201 | -     | 40,41,41     | 1.70 | 13 (32%) | 51,56,56    | 2.57 | 18 (35%) |
| 25  | CLA  | B     | 832 | -     | 62,66,73     | 1.24 | 9 (14%)  | 73,104,113  | 1.41 | 9 (12%)  |
| 28  | WVN  | l     | 315 | -     | 40,41,41     | 1.77 | 10 (25%) | 51,56,56    | 2.45 | 19 (37%) |
| 25  | CLA  | B     | 818 | 37    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.21 | 6 (7%)   |
| 25  | CLA  | m     | 612 | 37    | 55,59,73     | 1.30 | 6 (10%)  | 64,96,113   | 1.49 | 10 (15%) |
| 25  | CLA  | h     | 304 | -     | 55,59,73     | 1.27 | 7 (12%)  | 64,96,113   | 1.43 | 7 (10%)  |
| 25  | CLA  | i     | 308 | 20    | 55,59,73     | 1.29 | 7 (12%)  | 64,96,113   | 1.25 | 5 (7%)   |
| 32  | II0  | l     | 302 | -     | 39,43,43     | 6.82 | 23 (58%) | 48,60,60    | 1.96 | 14 (29%) |
| 25  | CLA  | B     | 839 | -     | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.31 | 8 (9%)   |
| 34  | KC2  | m     | 611 | 17    | 49,53,53     | 2.66 | 19 (38%) | 60,89,89    | 3.98 | 34 (56%) |
| 32  | II0  | n     | 315 | -     | 39,43,43     | 6.88 | 21 (53%) | 48,60,60    | 1.97 | 13 (27%) |
| 25  | CLA  | j     | 604 | 17    | 69,73,73     | 1.14 | 7 (10%)  | 82,113,113  | 1.35 | 9 (10%)  |
| 25  | CLA  | n     | 306 | 23    | 55,59,73     | 1.35 | 7 (12%)  | 64,96,113   | 1.55 | 9 (14%)  |
| 25  | CLA  | s     | 203 | 12,25 | 69,73,73     | 1.20 | 8 (11%)  | 82,113,113  | 1.38 | 9 (10%)  |
| 25  | CLA  | B     | 834 | -     | 51,55,73     | 1.28 | 6 (11%)  | 60,91,113   | 1.39 | 5 (8%)   |
| 25  | CLA  | s     | 206 | -     | 69,73,73     | 1.14 | 6 (8%)   | 82,113,113  | 1.48 | 11 (13%) |
| 25  | CLA  | B     | 817 | -     | 61,65,73     | 1.27 | 8 (13%)  | 72,103,113  | 1.47 | 11 (15%) |
| 32  | II0  | l     | 316 | -     | 39,43,43     | 6.58 | 21 (53%) | 48,60,60    | 1.90 | 12 (25%) |
| 34  | KC2  | i     | 319 | -     | 49,53,53     | 2.73 | 20 (40%) | 60,89,89    | 3.76 | 32 (53%) |
| 32  | II0  | c     | 615 | -     | 39,43,43     | 6.70 | 20 (51%) | 48,60,60    | 2.16 | 18 (37%) |
| 25  | CLA  | b     | 611 | -     | 69,73,73     | 1.14 | 6 (8%)   | 82,113,113  | 1.28 | 7 (8%)   |
| 25  | CLA  | A     | 823 | -     | 59,63,73     | 1.27 | 7 (11%)  | 70,101,113  | 1.33 | 6 (8%)   |
| 27  | LHG  | k     | 620 | 25    | 36,36,48     | 1.10 | 2 (5%)   | 39,42,54    | 1.20 | 4 (10%)  |
| 27  | LHG  | l     | 317 | 25    | 31,31,48     | 1.17 | 2 (6%)   | 34,37,54    | 1.22 | 3 (8%)   |
| 25  | CLA  | B     | 841 | 27    | 69,73,73     | 1.15 | 7 (10%)  | 82,113,113  | 1.37 | 7 (8%)   |
| 25  | CLA  | i     | 306 | -     | 55,59,73     | 1.31 | 6 (10%)  | 64,96,113   | 1.27 | 6 (9%)   |
| 32  | II0  | k     | 615 | -     | 39,43,43     | 6.69 | 21 (53%) | 48,60,60    | 1.81 | 11 (22%) |
| 25  | CLA  | B     | 838 | -     | 61,65,73     | 1.23 | 7 (11%)  | 72,103,113  | 1.33 | 6 (8%)   |
| 25  | CLA  | A     | 821 | -     | 53,57,73     | 1.27 | 6 (11%)  | 61,93,113   | 1.42 | 5 (8%)   |
| 25  | CLA  | n     | 303 | 23    | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.35 | 6 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | n     | 314 | -    | 55,59,73     | 1.28 | 7 (12%)  | 64,96,113   | 1.31 | 7 (10%)  |
| 25  | CLA  | A     | 842 | 37   | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.34 | 8 (9%)   |
| 27  | LHG  | a     | 301 | 25   | 48,48,48     | 0.96 | 3 (6%)   | 51,54,54    | 1.21 | 5 (9%)   |
| 27  | LHG  | J     | 106 | 25   | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 0.89 | 2 (3%)   |
| 25  | CLA  | A     | 814 | -    | 54,58,73     | 1.29 | 6 (11%)  | 64,95,113   | 1.43 | 7 (10%)  |
| 33  | LMG  | b     | 620 | -    | 49,49,55     | 0.95 | 3 (6%)   | 57,57,63    | 1.20 | 4 (7%)   |
| 25  | CLA  | B     | 822 | 37   | 69,73,73     | 1.21 | 11 (15%) | 82,113,113  | 1.48 | 14 (17%) |
| 25  | CLA  | d     | 309 | 27   | 45,49,73     | 1.38 | 6 (13%)  | 54,84,113   | 1.50 | 6 (11%)  |
| 27  | LHG  | c     | 620 | 25   | 36,36,48     | 1.01 | 2 (5%)   | 39,42,54    | 1.30 | 4 (10%)  |
| 28  | WVN  | B     | 846 | -    | 40,41,41     | 1.66 | 13 (32%) | 51,56,56    | 2.22 | 17 (33%) |
| 27  | LHG  | A     | 846 | 25   | 26,26,48     | 1.24 | 3 (11%)  | 29,32,54    | 1.40 | 6 (20%)  |
| 25  | CLA  | m     | 613 | -    | 47,51,73     | 1.38 | 8 (17%)  | 55,86,113   | 1.63 | 13 (23%) |
| 32  | II0  | n     | 317 | -    | 39,43,43     | 6.71 | 21 (53%) | 48,60,60    | 2.09 | 14 (29%) |
| 35  | IHT  | R     | 203 | -    | 40,42,42     | 6.26 | 25 (62%) | 52,58,58    | 2.38 | 17 (32%) |
| 25  | CLA  | h     | 306 | 16   | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.17 | 4 (4%)   |
| 28  | WVN  | A     | 851 | -    | 40,41,41     | 1.66 | 10 (25%) | 51,56,56    | 2.33 | 16 (31%) |
| 25  | CLA  | m     | 609 | 17   | 55,59,73     | 1.31 | 8 (14%)  | 64,96,113   | 1.30 | 7 (10%)  |
| 25  | CLA  | A     | 830 | -    | 54,58,73     | 1.33 | 9 (16%)  | 64,95,113   | 1.45 | 9 (14%)  |
| 32  | II0  | c     | 613 | -    | 39,43,43     | 6.74 | 22 (56%) | 48,60,60    | 1.89 | 14 (29%) |
| 25  | CLA  | a     | 312 | -    | 69,73,73     | 1.19 | 9 (13%)  | 82,113,113  | 1.66 | 9 (10%)  |
| 28  | WVN  | F     | 204 | -    | 40,41,41     | 1.76 | 12 (30%) | 51,56,56    | 3.02 | 19 (37%) |
| 25  | CLA  | i     | 311 | -    | 55,59,73     | 1.29 | 5 (9%)   | 64,96,113   | 1.32 | 4 (6%)   |
| 28  | WVN  | B     | 847 | -    | 40,41,41     | 1.68 | 9 (22%)  | 51,56,56    | 2.63 | 18 (35%) |
| 28  | WVN  | s     | 205 | -    | 40,41,41     | 1.62 | 14 (35%) | 51,56,56    | 2.61 | 23 (45%) |
| 25  | CLA  | h     | 302 | 16   | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.42 | 11 (17%) |
| 25  | CLA  | A     | 828 | -    | 69,73,73     | 1.19 | 9 (13%)  | 82,113,113  | 1.48 | 12 (14%) |
| 25  | CLA  | i     | 307 | 20   | 65,69,73     | 1.20 | 6 (9%)   | 77,108,113  | 1.36 | 9 (11%)  |
| 25  | CLA  | c     | 601 | 13   | 55,59,73     | 1.27 | 6 (10%)  | 64,96,113   | 1.34 | 6 (9%)   |
| 27  | LHG  | n     | 320 | -    | 42,42,48     | 1.01 | 2 (4%)   | 45,48,54    | 1.18 | 4 (8%)   |
| 25  | CLA  | l     | 307 | 18   | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.65 | 11 (13%) |
| 25  | CLA  | R     | 202 | -    | 55,59,73     | 1.30 | 6 (10%)  | 64,96,113   | 1.51 | 10 (15%) |
| 25  | CLA  | A     | 829 | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 25  | CLA  | A     | 856 | 27   | 45,49,73     | 1.48 | 6 (13%)  | 54,84,113   | 2.00 | 7 (12%)  |
| 27  | LHG  | j     | 617 | 25   | 29,29,48     | 1.22 | 2 (6%)   | 32,35,54    | 1.31 | 3 (9%)   |
| 28  | WVN  | I     | 101 | -    | 40,41,41     | 1.64 | 11 (27%) | 51,56,56    | 2.12 | 17 (33%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | B     | 840 | -    | 69,73,73     | 1.14 | 6 (8%)   | 82,113,113  | 1.40 | 8 (9%)   |
| 25  | CLA  | A     | 804 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.50 | 10 (12%) |
| 25  | CLA  | B     | 819 | -    | 50,54,73     | 1.32 | 8 (16%)  | 59,90,113   | 1.35 | 5 (8%)   |
| 33  | LMG  | s     | 208 | -    | 48,48,55     | 0.96 | 2 (4%)   | 56,56,63    | 1.28 | 5 (8%)   |
| 25  | CLA  | a     | 313 | -    | 52,56,73     | 1.29 | 7 (13%)  | 61,92,113   | 1.26 | 5 (8%)   |
| 25  | CLA  | i     | 303 | 20   | 54,58,73     | 1.27 | 8 (14%)  | 64,95,113   | 1.51 | 9 (14%)  |
| 25  | CLA  | B     | 828 | -    | 53,57,73     | 1.33 | 8 (15%)  | 61,93,113   | 1.50 | 10 (16%) |
| 25  | CLA  | b     | 603 | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.41 | 10 (12%) |
| 25  | CLA  | B     | 827 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.30 | 5 (7%)   |
| 25  | CLA  | A     | 839 | 37   | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.30 | 10 (12%) |
| 25  | CLA  | h     | 313 | 37   | 69,73,73     | 1.10 | 6 (8%)   | 82,113,113  | 1.27 | 5 (6%)   |
| 25  | CLA  | A     | 831 | -    | 69,73,73     | 1.17 | 6 (8%)   | 82,113,113  | 1.27 | 6 (7%)   |
| 25  | CLA  | B     | 813 | -    | 64,68,73     | 1.20 | 7 (10%)  | 76,107,113  | 1.34 | 7 (9%)   |
| 28  | WVN  | A     | 849 | -    | 40,41,41     | 1.60 | 14 (35%) | 51,56,56    | 2.32 | 22 (43%) |
| 32  | II0  | a     | 315 | -    | 39,43,43     | 6.54 | 21 (53%) | 48,60,60    | 2.03 | 18 (37%) |
| 32  | II0  | m     | 615 | -    | 39,43,43     | 6.50 | 22 (56%) | 48,60,60    | 2.15 | 20 (41%) |
| 25  | CLA  | A     | 801 | -    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.30 | 8 (9%)   |
| 25  | CLA  | L     | 202 | 9    | 53,57,73     | 1.30 | 6 (11%)  | 61,93,113   | 1.39 | 7 (11%)  |
| 25  | CLA  | k     | 601 | 19   | 55,59,73     | 1.32 | 6 (10%)  | 64,96,113   | 1.39 | 5 (7%)   |
| 25  | CLA  | A     | 820 | 37   | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.33 | 9 (10%)  |
| 27  | LHG  | c     | 618 | 25   | 36,36,48     | 1.09 | 2 (5%)   | 39,42,54    | 1.23 | 4 (10%)  |
| 25  | CLA  | Q     | 302 | 37   | 69,73,73     | 1.15 | 6 (8%)   | 82,113,113  | 1.20 | 5 (6%)   |
| 32  | II0  | c     | 617 | -    | 39,43,43     | 6.63 | 21 (53%) | 48,60,60    | 2.09 | 17 (35%) |
| 25  | CLA  | m     | 604 | 17   | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.33 | 10 (12%) |
| 32  | II0  | k     | 616 | -    | 39,43,43     | 6.61 | 21 (53%) | 48,60,60    | 2.25 | 19 (39%) |
| 25  | CLA  | j     | 603 | -    | 55,59,73     | 1.26 | 6 (10%)  | 64,96,113   | 1.46 | 8 (12%)  |
| 32  | II0  | k     | 617 | -    | 39,43,43     | 6.75 | 20 (51%) | 48,60,60    | 2.12 | 18 (37%) |
| 25  | CLA  | b     | 604 | 15   | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.38 | 8 (9%)   |
| 30  | SF4  | C     | 101 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 25  | CLA  | B     | 836 | -    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.51 | 8 (9%)   |
| 25  | CLA  | l     | 308 | 18   | 69,73,73     | 1.21 | 9 (13%)  | 82,113,113  | 1.36 | 8 (9%)   |
| 25  | CLA  | k     | 614 | -    | 55,59,73     | 1.33 | 6 (10%)  | 64,96,113   | 1.45 | 14 (21%) |
| 25  | CLA  | j     | 601 | 17   | 55,59,73     | 1.30 | 6 (10%)  | 64,96,113   | 1.30 | 5 (7%)   |
| 25  | CLA  | m     | 605 | 17   | 46,50,73     | 1.41 | 8 (17%)  | 53,85,113   | 1.41 | 6 (11%)  |
| 35  | IHT  | a     | 317 | -    | 40,42,42     | 6.24 | 26 (65%) | 52,58,58    | 2.05 | 15 (28%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | II0  | a     | 314 | -    | 39,43,43     | 6.59 | 23 (58%) | 48,60,60    | 1.87 | 15 (31%) |
| 25  | CLA  | c     | 605 | 13   | 55,59,73     | 1.35 | 7 (12%)  | 64,96,113   | 1.37 | 7 (10%)  |
| 25  | CLA  | A     | 815 | 37   | 49,53,73     | 1.38 | 6 (12%)  | 58,89,113   | 1.49 | 8 (13%)  |
| 25  | CLA  | A     | 824 | 37   | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.33 | 8 (9%)   |
| 34  | KC2  | s     | 201 | 12   | 49,53,53     | 2.59 | 20 (40%) | 60,89,89    | 3.83 | 33 (55%) |
| 35  | IHT  | c     | 616 | -    | 40,42,42     | 6.14 | 25 (62%) | 52,58,58    | 2.33 | 16 (30%) |
| 25  | CLA  | A     | 806 | -    | 69,73,73     | 1.14 | 6 (8%)   | 82,113,113  | 1.28 | 7 (8%)   |
| 35  | IHT  | j     | 616 | -    | 40,42,42     | 6.22 | 26 (65%) | 52,58,58    | 2.41 | 16 (30%) |
| 32  | II0  | c     | 614 | -    | 39,43,43     | 6.57 | 20 (51%) | 48,60,60    | 2.16 | 14 (29%) |
| 25  | CLA  | A     | 813 | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.44 | 9 (15%)  |
| 32  | II0  | l     | 313 | -    | 39,43,43     | 6.79 | 22 (56%) | 48,60,60    | 1.70 | 11 (22%) |
| 32  | II0  | n     | 319 | -    | 39,43,43     | 6.72 | 20 (51%) | 48,60,60    | 1.73 | 11 (22%) |
| 32  | II0  | b     | 617 | -    | 39,43,43     | 6.72 | 21 (53%) | 48,60,60    | 2.14 | 15 (31%) |
| 25  | CLA  | B     | 829 | -    | 54,58,73     | 1.29 | 7 (12%)  | 64,95,113   | 1.34 | 6 (9%)   |
| 30  | SF4  | C     | 102 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 25  | CLA  | a     | 304 | 14   | 54,58,73     | 1.44 | 9 (16%)  | 64,95,113   | 1.46 | 11 (17%) |
| 25  | CLA  | B     | 823 | 37   | 68,72,73     | 1.19 | 9 (13%)  | 80,111,113  | 1.46 | 15 (18%) |
| 25  | CLA  | m     | 607 | -    | 55,59,73     | 1.44 | 11 (20%) | 64,96,113   | 1.71 | 16 (25%) |
| 35  | IHT  | k     | 618 | -    | 40,42,42     | 6.22 | 25 (62%) | 52,58,58    | 2.27 | 14 (26%) |
| 34  | KC2  | j     | 610 | 17   | 49,53,53     | 2.69 | 20 (40%) | 60,89,89    | 3.96 | 34 (56%) |
| 25  | CLA  | j     | 606 | -    | 55,59,73     | 1.27 | 7 (12%)  | 64,96,113   | 1.53 | 6 (9%)   |
| 25  | CLA  | d     | 301 | 21   | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.42 | 9 (14%)  |
| 25  | CLA  | L     | 204 | -    | 54,58,73     | 1.32 | 6 (11%)  | 64,95,113   | 1.41 | 7 (10%)  |
| 25  | CLA  | A     | 835 | -    | 69,73,73     | 1.14 | 7 (10%)  | 82,113,113  | 1.23 | 7 (8%)   |
| 27  | LHG  | d     | 317 | 25   | 36,36,48     | 1.10 | 2 (5%)   | 39,42,54    | 1.01 | 2 (5%)   |
| 35  | IHT  | n     | 318 | -    | 40,42,42     | 6.23 | 25 (62%) | 52,58,58    | 2.38 | 16 (30%) |
| 32  | II0  | m     | 618 | -    | 39,43,43     | 6.41 | 21 (53%) | 48,60,60    | 2.38 | 20 (41%) |
| 25  | CLA  | A     | 807 | 1    | 69,73,73     | 1.12 | 6 (8%)   | 82,113,113  | 1.34 | 7 (8%)   |
| 32  | II0  | J     | 104 | -    | 39,43,43     | 6.56 | 21 (53%) | 48,60,60    | 2.15 | 13 (27%) |
| 25  | CLA  | A     | 836 | -    | 69,73,73     | 1.17 | 6 (8%)   | 82,113,113  | 1.41 | 9 (10%)  |
| 25  | CLA  | l     | 304 | 18   | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.25 | 9 (10%)  |
| 25  | CLA  | L     | 203 | -    | 69,73,73     | 1.15 | 7 (10%)  | 82,113,113  | 1.26 | 7 (8%)   |
| 25  | CLA  | i     | 305 | 20   | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.38 | 9 (10%)  |
| 25  | CLA  | A     | 808 | 1    | 69,73,73     | 1.15 | 7 (10%)  | 82,113,113  | 1.34 | 10 (12%) |
| 25  | CLA  | A     | 826 | -    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.50 | 8 (9%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | A     | 818 | -    | 69,73,73     | 1.21 | 7 (10%)  | 82,113,113  | 1.62 | 16 (19%) |
| 25  | CLA  | B     | 811 | -    | 59,63,73     | 1.27 | 7 (11%)  | 70,101,113  | 1.43 | 8 (11%)  |
| 25  | CLA  | b     | 608 | 27   | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 25  | CLA  | k     | 602 | 19   | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.62 | 13 (20%) |
| 25  | CLA  | A     | 802 | -    | 69,73,73     | 1.19 | 9 (13%)  | 82,113,113  | 1.57 | 13 (15%) |
| 25  | CLA  | a     | 308 | 14   | 69,73,73     | 1.16 | 5 (7%)   | 82,113,113  | 1.27 | 12 (14%) |
| 25  | CLA  | n     | 305 | 23   | 64,68,73     | 1.21 | 7 (10%)  | 76,107,113  | 1.33 | 10 (13%) |
| 32  | II0  | d     | 314 | -    | 39,43,43     | 6.84 | 22 (56%) | 48,60,60    | 1.98 | 11 (22%) |
| 28  | WVN  | h     | 309 | -    | 40,41,41     | 1.76 | 10 (25%) | 51,56,56    | 2.28 | 19 (37%) |
| 25  | CLA  | n     | 302 | 23   | 49,53,73     | 1.37 | 6 (12%)  | 58,89,113   | 1.32 | 3 (5%)   |
| 34  | KC2  | k     | 613 | 34   | 49,53,53     | 2.78 | 20 (40%) | 60,89,89    | 3.64 | 33 (55%) |
| 28  | WVN  | B     | 844 | -    | 40,41,41     | 1.76 | 10 (25%) | 51,56,56    | 2.43 | 18 (35%) |
| 25  | CLA  | d     | 302 | -    | 55,59,73     | 1.27 | 6 (10%)  | 64,96,113   | 1.62 | 11 (17%) |
| 28  | WVN  | A     | 847 | -    | 40,41,41     | 1.69 | 12 (30%) | 51,56,56    | 2.18 | 15 (29%) |
| 28  | WVN  | l     | 301 | -    | 40,41,41     | 1.67 | 10 (25%) | 51,56,56    | 2.35 | 19 (37%) |
| 25  | CLA  | k     | 604 | -    | 69,73,73     | 1.14 | 8 (11%)  | 82,113,113  | 1.30 | 9 (10%)  |
| 28  | WVN  | L     | 206 | -    | 40,41,41     | 1.67 | 12 (30%) | 51,56,56    | 2.75 | 22 (43%) |
| 25  | CLA  | n     | 304 | -    | 55,59,73     | 1.35 | 8 (14%)  | 64,96,113   | 1.66 | 13 (20%) |
| 28  | WVN  | J     | 102 | -    | 40,41,41     | 1.62 | 12 (30%) | 51,56,56    | 2.30 | 19 (37%) |
| 25  | CLA  | B     | 815 | -    | 59,63,73     | 1.24 | 6 (10%)  | 70,101,113  | 1.35 | 9 (12%)  |
| 34  | KC2  | d     | 311 | -    | 49,53,53     | 2.80 | 20 (40%) | 60,89,89    | 3.59 | 33 (55%) |
| 25  | CLA  | h     | 305 | 16   | 55,59,73     | 1.27 | 6 (10%)  | 64,96,113   | 1.36 | 7 (10%)  |
| 25  | CLA  | A     | 816 | -    | 69,73,73     | 1.14 | 5 (7%)   | 82,113,113  | 1.39 | 10 (12%) |
| 25  | CLA  | Q     | 303 | 24   | 49,53,73     | 1.35 | 8 (16%)  | 58,89,113   | 1.45 | 9 (15%)  |
| 25  | CLA  | h     | 303 | 16   | 54,58,73     | 1.33 | 9 (16%)  | 64,95,113   | 1.46 | 8 (12%)  |
| 29  | LMT  | a     | 302 | -    | 24,24,36     | 1.15 | 3 (12%)  | 29,29,47    | 0.99 | 2 (6%)   |
| 25  | CLA  | B     | 826 | -    | 69,73,73     | 1.17 | 10 (14%) | 82,113,113  | 1.21 | 8 (9%)   |
| 32  | II0  | l     | 314 | -    | 39,43,43     | 6.71 | 20 (51%) | 48,60,60    | 2.67 | 14 (29%) |
| 32  | II0  | a     | 316 | -    | 39,43,43     | 6.48 | 20 (51%) | 48,60,60    | 2.36 | 15 (31%) |
| 25  | CLA  | A     | 811 | -    | 58,62,73     | 1.26 | 6 (10%)  | 68,99,113   | 1.40 | 7 (10%)  |
| 25  | CLA  | A     | 834 | -    | 55,59,73     | 1.31 | 8 (14%)  | 64,96,113   | 1.47 | 11 (17%) |
| 25  | CLA  | m     | 610 | 27   | 59,63,73     | 1.22 | 6 (10%)  | 70,101,113  | 1.42 | 7 (10%)  |
| 25  | CLA  | A     | 841 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 25  | CLA  | j     | 602 | 17   | 54,58,73     | 1.32 | 7 (12%)  | 64,95,113   | 1.47 | 8 (12%)  |
| 25  | CLA  | B     | 830 | 37   | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.30 | 8 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 27  | LHG  | J     | 107 | -    | 30,30,48     | 1.14 | 2 (6%)   | 33,36,54    | 1.21 | 4 (12%)  |
| 25  | CLA  | A     | 838 | 27   | 56,60,73     | 1.26 | 7 (12%)  | 65,97,113   | 1.33 | 7 (10%)  |
| 25  | CLA  | s     | 209 | -    | 55,59,73     | 1.27 | 6 (10%)  | 64,96,113   | 1.49 | 6 (9%)   |
| 25  | CLA  | n     | 308 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.46 | 16 (19%) |
| 28  | WVN  | F     | 203 | -    | 40,41,41     | 1.71 | 13 (32%) | 51,56,56    | 2.84 | 23 (45%) |
| 25  | CLA  | c     | 609 | 27   | 49,53,73     | 1.35 | 5 (10%)  | 58,89,113   | 1.34 | 5 (8%)   |
| 29  | LMT  | b     | 618 | -    | 24,24,36     | 1.04 | 2 (8%)   | 29,29,47    | 0.95 | 0        |
| 25  | CLA  | c     | 611 | -    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.54 | 6 (10%)  |
| 29  | LMT  | A     | 852 | -    | 36,36,36     | 0.39 | 0        | 47,47,47    | 0.93 | 3 (6%)   |
| 35  | IHT  | b     | 616 | -    | 40,42,42     | 6.25 | 26 (65%) | 52,58,58    | 2.88 | 16 (30%) |
| 28  | WVN  | B     | 849 | -    | 40,41,41     | 1.71 | 11 (27%) | 51,56,56    | 2.16 | 16 (31%) |
| 34  | KC2  | n     | 312 | 23   | 49,53,53     | 2.67 | 19 (38%) | 60,89,89    | 3.91 | 36 (60%) |
| 25  | CLA  | a     | 309 | 14   | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.60 | 10 (12%) |
| 25  | CLA  | B     | 814 | -    | 63,67,73     | 1.18 | 7 (11%)  | 74,105,113  | 1.44 | 7 (9%)   |
| 25  | CLA  | m     | 608 | 17   | 69,73,73     | 1.22 | 8 (11%)  | 82,113,113  | 1.24 | 9 (10%)  |
| 32  | II0  | k     | 619 | -    | 39,43,43     | 6.70 | 21 (53%) | 48,60,60    | 2.14 | 17 (35%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 28  | WVN  | i     | 316 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 32  | II0  | d     | 315 | -    | -         | 6/21/67/67    | 0/2/2/2 |
| 25  | CLA  | A     | 853 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 25  | CLA  | K     | 102 | -    | 1/1/10/20 | 4/12/88/115   | -       |
| 28  | WVN  | A     | 848 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 28  | WVN  | R     | 201 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 25  | CLA  | l     | 309 | 18   | 1/1/12/20 | 6/23/99/115   | -       |
| 25  | CLA  | F     | 201 | 37   | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | CLA  | d     | 306 | -    | 1/1/12/20 | 9/23/99/115   | -       |
| 25  | CLA  | A     | 805 | 1    | 1/1/15/20 | 9/39/115/115  | -       |
| 28  | WVN  | J     | 101 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 25  | CLA  | J     | 103 | 8    | 1/1/10/20 | 5/12/88/115   | -       |
| 36  | LMU  | i     | 301 | -    | -         | 9/21/61/61    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | B     | 804 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 25  | CLA  | A     | 825 | 37   | -         | 9/39/115/115  | -       |
| 34  | KC2  | s     | 204 | -    | -         | 6/15/71/71    | -       |
| 25  | CLA  | A     | 854 | -    | 1/1/15/20 | 20/39/115/115 | -       |
| 32  | II0  | a     | 318 | -    | -         | 7/21/67/67    | 0/2/2/2 |
| 25  | CLA  | j     | 607 | 17   | 1/1/11/20 | 6/15/91/115   | -       |
| 25  | CLA  | B     | 835 | 37   | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | CLA  | c     | 606 | -    | -         | 11/24/100/115 | -       |
| 25  | CLA  | n     | 307 | 23   | 1/1/12/20 | 6/23/99/115   | -       |
| 33  | LMG  | J     | 105 | -    | -         | 14/50/70/70   | 0/1/1/1 |
| 32  | II0  | j     | 614 | -    | -         | 4/21/67/67    | 0/2/2/2 |
| 25  | CLA  | d     | 303 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 25  | CLA  | B     | 837 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 25  | CLA  | B     | 806 | -    | 1/1/15/20 | 22/39/115/115 | -       |
| 25  | CLA  | a     | 307 | 14   | -         | 9/15/91/115   | -       |
| 32  | II0  | h     | 310 | -    | -         | 2/17/40/67    | 0/1/1/2 |
| 25  | CLA  | k     | 605 | 19   | 1/1/11/20 | 7/15/91/115   | -       |
| 25  | CLA  | l     | 306 | 18   | -         | 18/39/115/115 | -       |
| 34  | KC2  | d     | 310 | 21   | -         | 8/15/71/71    | -       |
| 25  | CLA  | B     | 820 | -    | -         | 12/27/103/115 | -       |
| 32  | II0  | n     | 301 | -    | -         | 4/21/67/67    | 0/2/2/2 |
| 25  | CLA  | c     | 604 | 13   | 1/1/15/20 | 18/39/115/115 | -       |
| 27  | LHG  | m     | 617 | 25   | -         | 16/41/41/53   | -       |
| 30  | SF4  | B     | 802 | -    | -         | -             | 0/6/5/5 |
| 34  | KC2  | n     | 313 | -    | -         | 7/15/71/71    | -       |
| 25  | CLA  | l     | 310 | 27   | 1/1/14/20 | 14/35/111/115 | -       |
| 25  | CLA  | F     | 202 | 6    | -         | 10/24/100/115 | -       |
| 28  | WVN  | A     | 850 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 25  | CLA  | b     | 609 | -    | -         | 5/23/99/115   | -       |
| 28  | WVN  | M     | 101 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 25  | CLA  | A     | 803 | -    | -         | 8/27/103/115  | -       |
| 32  | II0  | i     | 320 | -    | -         | 6/21/67/67    | 0/2/2/2 |
| 34  | KC2  | i     | 310 | 20   | -         | 9/15/71/71    | -       |
| 25  | CLA  | s     | 202 | 12   | 1/1/15/20 | 17/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 29  | LMT  | a     | 320 | -    | -         | 9/21/61/61    | 0/2/2/2 |
| 25  | CLA  | b     | 601 | 15   | 1/1/12/20 | 9/23/99/115   | -       |
| 25  | CLA  | A     | 833 | -    | 1/1/12/20 | 7/21/97/115   | -       |
| 27  | LHG  | A     | 845 | -    | -         | 22/52/52/53   | -       |
| 32  | II0  | i     | 314 | -    | -         | 5/21/67/67    | 0/2/2/2 |
| 25  | CLA  | d     | 307 | -    | 1/1/11/20 | 5/17/93/115   | -       |
| 25  | CLA  | c     | 608 | 13   | 1/1/15/20 | 16/39/115/115 | -       |
| 28  | WVN  | s     | 207 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 25  | CLA  | b     | 602 | 15   | 1/1/13/20 | 13/27/103/115 | -       |
| 25  | CLA  | n     | 311 | 37   | -         | 15/39/115/115 | -       |
| 32  | II0  | h     | 311 | -    | -         | 7/21/67/67    | 0/2/2/2 |
| 25  | CLA  | B     | 850 | -    | 1/1/12/20 | 4/23/99/115   | -       |
| 25  | CLA  | k     | 607 | -    | 1/1/12/20 | 10/23/99/115  | -       |
| 25  | CLA  | m     | 601 | 17   | 1/1/10/20 | 2/12/88/115   | -       |
| 25  | CLA  | B     | 803 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 25  | CLA  | A     | 812 | -    | 1/1/15/20 | 25/39/115/115 | -       |
| 25  | CLA  | m     | 606 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | CLA  | A     | 855 | 37   | 1/1/15/20 | 26/39/115/115 | -       |
| 34  | KC2  | k     | 612 | 34   | -         | 8/15/71/71    | -       |
| 25  | CLA  | i     | 302 | 20   | 1/1/12/20 | 8/23/99/115   | -       |
| 25  | CLA  | A     | 819 | -    | -         | 7/15/91/115   | -       |
| 25  | CLA  | n     | 309 | 23   | 1/1/12/20 | 7/23/99/115   | -       |
| 25  | CLA  | B     | 831 | 37   | -         | 4/15/91/115   | -       |
| 25  | CLA  | a     | 310 | 27   | 1/1/11/20 | 8/19/95/115   | -       |
| 32  | II0  | m     | 614 | -    | -         | 3/21/67/67    | 0/2/2/2 |
| 25  | CLA  | A     | 843 | -    | 1/1/15/20 | 22/39/115/115 | -       |
| 25  | CLA  | B     | 810 | -    | 1/1/13/20 | 3/25/101/115  | -       |
| 25  | CLA  | l     | 305 | -    | 1/1/12/20 | 2/23/99/115   | -       |
| 25  | CLA  | a     | 306 | 37   | 1/1/15/20 | 13/39/115/115 | -       |
| 35  | IHT  | b     | 615 | -    | -         | 6/25/65/65    | 0/2/2/2 |
| 27  | LHG  | L     | 207 | -    | -         | 22/53/53/53   | -       |
| 25  | CLA  | c     | 612 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 25  | CLA  | j     | 609 | 27   | 1/1/14/20 | 14/35/111/115 | -       |
| 25  | CLA  | h     | 307 | 16   | 1/1/13/20 | 9/30/106/115  | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 25  | CLA  | k     | 608 | 19    | 1/1/15/20 | 16/39/115/115 | -       |
| 25  | CLA  | k     | 610 | 27    | 1/1/12/20 | 10/23/99/115  | -       |
| 34  | KC2  | l     | 311 | 18    | -         | 11/15/71/71   | -       |
| 25  | CLA  | c     | 607 | 13    | 1/1/11/20 | 5/17/93/115   | -       |
| 25  | CLA  | a     | 305 | -     | 1/1/12/20 | 7/23/99/115   | -       |
| 25  | CLA  | b     | 605 | 37,25 | 1/1/15/20 | 12/39/115/115 | -       |
| 25  | CLA  | k     | 606 | 19    | -         | 12/23/99/115  | -       |
| 25  | CLA  | h     | 301 | 37    | -         | 15/39/115/115 | -       |
| 35  | IHT  | m     | 616 | -     | -         | 7/25/65/65    | 0/2/2/2 |
| 25  | CLA  | B     | 808 | -     | 1/1/15/20 | 16/39/115/115 | -       |
| 32  | II0  | h     | 312 | -     | -         | 7/21/67/67    | 0/2/2/2 |
| 25  | CLA  | A     | 840 | 1     | -         | 16/39/115/115 | -       |
| 25  | CLA  | B     | 833 | -     | 1/1/15/20 | 15/39/115/115 | -       |
| 25  | CLA  | A     | 822 | -     | -         | 10/23/99/115  | -       |
| 25  | CLA  | m     | 603 | -     | 1/1/15/20 | 21/39/115/115 | -       |
| 32  | II0  | j     | 613 | -     | -         | 7/21/67/67    | 0/2/2/2 |
| 25  | CLA  | j     | 612 | -     | 1/1/15/20 | 12/39/115/115 | -       |
| 32  | II0  | d     | 313 | -     | -         | 7/21/67/67    | 0/2/2/2 |
| 25  | CLA  | i     | 309 | 27    | 1/1/11/20 | 6/17/93/115   | -       |
| 25  | CLA  | B     | 812 | -     | 1/1/15/20 | 19/39/115/115 | -       |
| 27  | LHG  | B     | 801 | -     | -         | 27/42/42/53   | -       |
| 33  | LMG  | n     | 321 | -     | -         | 9/50/70/70    | 0/1/1/1 |
| 25  | CLA  | b     | 607 | 15    | 1/1/15/20 | 15/39/115/115 | -       |
| 25  | CLA  | n     | 310 | 23    | 1/1/15/20 | 15/39/115/115 | -       |
| 27  | LHG  | a     | 319 | 25    | -         | 16/53/53/53   | -       |
| 25  | CLA  | a     | 311 | 14    | 1/1/15/20 | 12/39/115/115 | -       |
| 25  | CLA  | A     | 837 | -     | 1/1/15/20 | 18/39/115/115 | -       |
| 32  | II0  | i     | 313 | -     | -         | 6/21/67/67    | 0/2/2/2 |
| 25  | CLA  | B     | 825 | -     | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | CLA  | i     | 312 | -     | 1/1/12/20 | 7/23/99/115   | -       |
| 26  | PQN  | A     | 844 | -     | -         | 9/23/43/43    | 0/2/2/2 |
| 25  | CLA  | B     | 816 | -     | 1/1/13/20 | 12/32/108/115 | -       |
| 25  | CLA  | B     | 824 | -     | 1/1/15/20 | 12/39/115/115 | -       |
| 25  | CLA  | l     | 312 | 18    | 1/1/15/20 | 13/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | B     | 805 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 28  | WVN  | K     | 103 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 25  | CLA  | h     | 308 | 16   | 1/1/12/20 | 10/23/99/115  | -       |
| 25  | CLA  | c     | 602 | 13   | 1/1/12/20 | 9/21/97/115   | -       |
| 32  | II0  | n     | 316 | -    | -         | 3/21/67/67    | 0/2/2/2 |
| 25  | CLA  | k     | 603 | -    | 1/1/12/20 | 5/23/99/115   | -       |
| 32  | II0  | j     | 615 | -    | -         | 9/21/67/67    | 0/2/2/2 |
| 28  | WVN  | L     | 205 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 32  | II0  | i     | 315 | -    | -         | 5/21/67/67    | 0/2/2/2 |
| 25  | CLA  | B     | 809 | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 25  | CLA  | d     | 305 | 21   | 1/1/12/20 | 7/23/99/115   | -       |
| 25  | CLA  | m     | 602 | 17   | 1/1/13/20 | 11/29/105/115 | -       |
| 25  | CLA  | A     | 827 | -    | -         | 14/36/112/115 | -       |
| 25  | CLA  | B     | 821 | -    | -         | 9/25/101/115  | -       |
| 28  | WVN  | B     | 848 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 25  | CLA  | j     | 611 | -    | 1/1/12/20 | 9/23/99/115   | -       |
| 25  | CLA  | j     | 605 | 17   | 1/1/11/20 | 8/15/91/115   | -       |
| 25  | CLA  | l     | 303 | 18   | 1/1/11/20 | 8/18/94/115   | -       |
| 25  | CLA  | d     | 304 | 21   | 1/1/12/20 | 8/23/99/115   | -       |
| 31  | DGD  | B     | 843 | -    | -         | 5/49/89/95    | 0/2/2/2 |
| 25  | CLA  | b     | 606 | 15   | 1/1/14/20 | 12/35/111/115 | -       |
| 25  | CLA  | K     | 101 | 37   | 1/1/12/20 | 8/23/99/115   | -       |
| 25  | CLA  | A     | 832 | -    | -         | 13/39/115/115 | -       |
| 26  | PQN  | B     | 842 | -    | -         | 12/23/43/43   | 0/2/2/2 |
| 25  | CLA  | b     | 610 | 15   | 1/1/15/20 | 18/39/115/115 | -       |
| 34  | KC2  | c     | 610 | -    | -         | 9/15/71/71    | -       |
| 25  | CLA  | a     | 303 | 14   | 1/1/12/20 | 10/24/100/115 | -       |
| 25  | CLA  | A     | 817 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 25  | CLA  | c     | 603 | -    | 1/1/12/20 | 7/23/99/115   | -       |
| 25  | CLA  | A     | 810 | -    | 1/1/14/20 | 10/36/112/115 | -       |
| 25  | CLA  | i     | 304 | -    | 1/1/12/20 | 7/23/99/115   | -       |
| 32  | II0  | d     | 316 | -    | -         | 6/21/67/67    | 0/2/2/2 |
| 33  | LMG  | Q     | 301 | -    | -         | 10/33/53/70   | 0/1/1/1 |
| 25  | CLA  | A     | 809 | -    | -         | 12/29/105/115 | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 34  | KC2  | k     | 611 | 19    | -         | 9/15/71/71    | -       |
| 25  | CLA  | d     | 312 | -     | 1/1/12/20 | 8/23/99/115   | -       |
| 27  | LHG  | b     | 619 | 25    | -         | 21/53/53/53   | -       |
| 32  | II0  | i     | 317 | -     | -         | 6/21/67/67    | 0/2/2/2 |
| 33  | LMG  | c     | 619 | -     | -         | 20/50/70/70   | 0/1/1/1 |
| 25  | CLA  | d     | 308 | 21    | 1/1/10/20 | 2/10/86/115   | -       |
| 28  | WVN  | B     | 845 | -     | -         | 0/29/63/63    | 0/2/2/2 |
| 32  | II0  | b     | 613 | -     | -         | 2/21/67/67    | 0/2/2/2 |
| 25  | CLA  | B     | 807 | -     | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | CLA  | b     | 612 | 27    | -         | 6/23/99/115   | -       |
| 25  | CLA  | k     | 609 | 19    | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | CLA  | j     | 608 | 17    | 1/1/12/20 | 0/23/99/115   | -       |
| 32  | II0  | b     | 614 | -     | -         | 8/21/67/67    | 0/2/2/2 |
| 27  | LHG  | i     | 318 | 25    | -         | 11/41/41/53   | -       |
| 28  | WVN  | L     | 201 | -     | -         | 8/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B     | 832 | -     | 1/1/13/20 | 10/31/107/115 | -       |
| 28  | WVN  | l     | 315 | -     | -         | 9/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B     | 818 | 37    | 1/1/15/20 | 18/39/115/115 | -       |
| 25  | CLA  | m     | 612 | 37    | -         | 10/23/99/115  | -       |
| 25  | CLA  | h     | 304 | -     | 1/1/12/20 | 6/23/99/115   | -       |
| 25  | CLA  | i     | 308 | 20    | 1/1/12/20 | 11/23/99/115  | -       |
| 32  | II0  | l     | 302 | -     | -         | 8/21/67/67    | 0/2/2/2 |
| 25  | CLA  | B     | 839 | -     | 1/1/15/20 | 19/39/115/115 | -       |
| 34  | KC2  | m     | 611 | 17    | -         | 6/15/71/71    | -       |
| 32  | II0  | n     | 315 | -     | -         | 1/21/67/67    | 0/2/2/2 |
| 25  | CLA  | j     | 604 | 17    | -         | 13/39/115/115 | -       |
| 25  | CLA  | n     | 306 | 23    | 1/1/12/20 | 6/23/99/115   | -       |
| 25  | CLA  | s     | 203 | 12,25 | -         | 13/39/115/115 | -       |
| 25  | CLA  | B     | 834 | -     | 1/1/11/20 | 3/18/94/115   | -       |
| 25  | CLA  | s     | 206 | -     | -         | 15/39/115/115 | -       |
| 25  | CLA  | B     | 817 | -     | 1/1/13/20 | 11/30/106/115 | -       |
| 32  | II0  | l     | 316 | -     | -         | 5/21/67/67    | 0/2/2/2 |
| 34  | KC2  | i     | 319 | -     | -         | 7/15/71/71    | -       |
| 32  | II0  | c     | 615 | -     | -         | 3/21/67/67    | 0/2/2/2 |
| 25  | CLA  | b     | 611 | -     | 1/1/15/20 | 17/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | A     | 823 | -    | -         | 14/27/103/115 | -       |
| 27  | LHG  | k     | 620 | 25   | -         | 9/41/41/53    | -       |
| 27  | LHG  | l     | 317 | 25   | -         | 14/36/36/53   | -       |
| 25  | CLA  | B     | 841 | 27   | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | CLA  | i     | 306 | -    | 1/1/12/20 | 10/23/99/115  | -       |
| 32  | II0  | k     | 615 | -    | -         | 6/21/67/67    | 0/2/2/2 |
| 25  | CLA  | B     | 838 | -    | -         | 12/30/106/115 | -       |
| 25  | CLA  | n     | 303 | 23   | 1/1/12/20 | 7/21/97/115   | -       |
| 25  | CLA  | A     | 821 | -    | -         | 9/20/96/115   | -       |
| 25  | CLA  | n     | 314 | -    | -         | 11/23/99/115  | -       |
| 25  | CLA  | A     | 842 | 37   | 1/1/15/20 | 16/39/115/115 | -       |
| 27  | LHG  | a     | 301 | 25   | -         | 13/53/53/53   | -       |
| 27  | LHG  | J     | 106 | 25   | -         | 20/53/53/53   | -       |
| 25  | CLA  | A     | 814 | -    | -         | 7/21/97/115   | -       |
| 33  | LMG  | b     | 620 | -    | -         | 17/44/64/70   | 0/1/1/1 |
| 25  | CLA  | B     | 822 | 37   | 1/1/15/20 | 17/39/115/115 | -       |
| 25  | CLA  | d     | 309 | 27   | 1/1/10/20 | 4/10/86/115   | -       |
| 27  | LHG  | c     | 620 | 25   | -         | 25/41/41/53   | -       |
| 28  | WVN  | B     | 846 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 27  | LHG  | A     | 846 | 25   | -         | 6/31/31/53    | -       |
| 25  | CLA  | m     | 613 | -    | 1/1/10/20 | 8/13/89/115   | -       |
| 32  | II0  | n     | 317 | -    | -         | 3/21/67/67    | 0/2/2/2 |
| 35  | IHT  | R     | 203 | -    | -         | 4/25/65/65    | 0/2/2/2 |
| 25  | CLA  | h     | 306 | 16   | 1/1/15/20 | 13/39/115/115 | -       |
| 28  | WVN  | A     | 851 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 25  | CLA  | m     | 609 | 17   | 1/1/12/20 | 8/23/99/115   | -       |
| 25  | CLA  | A     | 830 | -    | -         | 7/21/97/115   | -       |
| 32  | II0  | c     | 613 | -    | -         | 4/21/67/67    | 0/2/2/2 |
| 25  | CLA  | a     | 312 | -    | -         | 20/39/115/115 | -       |
| 28  | WVN  | F     | 204 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 25  | CLA  | i     | 311 | -    | 1/1/12/20 | 13/23/99/115  | -       |
| 28  | WVN  | B     | 847 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 28  | WVN  | s     | 205 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 25  | CLA  | h     | 302 | 16   | 1/1/12/20 | 8/21/97/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | A     | 828 | -    | -         | 6/39/115/115  | -       |
| 25  | CLA  | i     | 307 | 20   | 1/1/14/20 | 12/35/111/115 | -       |
| 25  | CLA  | c     | 601 | 13   | 1/1/12/20 | 12/23/99/115  | -       |
| 27  | LHG  | n     | 320 | -    | -         | 16/47/47/53   | -       |
| 25  | CLA  | l     | 307 | 18   | 1/1/15/20 | 17/39/115/115 | -       |
| 25  | CLA  | R     | 202 | -    | 1/1/12/20 | 12/23/99/115  | -       |
| 25  | CLA  | A     | 829 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 25  | CLA  | A     | 856 | 27   | 1/1/10/20 | 4/10/86/115   | -       |
| 27  | LHG  | j     | 617 | 25   | -         | 5/34/34/53    | -       |
| 28  | WVN  | I     | 101 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B     | 840 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 25  | CLA  | A     | 804 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 25  | CLA  | B     | 819 | -    | -         | 6/17/93/115   | -       |
| 33  | LMG  | s     | 208 | -    | -         | 11/43/63/70   | 0/1/1/1 |
| 25  | CLA  | a     | 313 | -    | 1/1/11/20 | 11/19/95/115  | -       |
| 25  | CLA  | i     | 303 | 20   | 1/1/12/20 | 11/21/97/115  | -       |
| 25  | CLA  | b     | 603 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 25  | CLA  | B     | 828 | -    | -         | 5/20/96/115   | -       |
| 25  | CLA  | B     | 827 | -    | -         | 8/21/97/115   | -       |
| 25  | CLA  | A     | 839 | 37   | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | CLA  | h     | 313 | 37   | 1/1/15/20 | 8/39/115/115  | -       |
| 25  | CLA  | A     | 831 | -    | -         | 14/39/115/115 | -       |
| 25  | CLA  | B     | 813 | -    | 1/1/14/20 | 15/33/109/115 | -       |
| 28  | WVN  | A     | 849 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 32  | II0  | a     | 315 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 32  | II0  | m     | 615 | -    | -         | 7/21/67/67    | 0/2/2/2 |
| 25  | CLA  | A     | 801 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 25  | CLA  | L     | 202 | 9    | 1/1/11/20 | 8/20/96/115   | -       |
| 25  | CLA  | k     | 601 | 19   | 1/1/12/20 | 7/23/99/115   | -       |
| 25  | CLA  | A     | 820 | 37   | 1/1/15/20 | 15/39/115/115 | -       |
| 27  | LHG  | c     | 618 | 25   | -         | 14/41/41/53   | -       |
| 25  | CLA  | Q     | 302 | 37   | 1/1/15/20 | 15/39/115/115 | -       |
| 32  | II0  | c     | 617 | -    | -         | 4/21/67/67    | 0/2/2/2 |
| 25  | CLA  | m     | 604 | 17   | -         | 16/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 32  | II0  | k     | 616 | -    | -         | 8/21/67/67    | 0/2/2/2 |
| 25  | CLA  | j     | 603 | -    | 1/1/12/20 | 7/23/99/115   | -       |
| 32  | II0  | k     | 617 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 25  | CLA  | b     | 604 | 15   | -         | 17/39/115/115 | -       |
| 30  | SF4  | C     | 101 | 3    | -         | -             | 0/6/5/5 |
| 25  | CLA  | B     | 836 | -    | -         | 23/39/115/115 | -       |
| 25  | CLA  | l     | 308 | 18   | 1/1/15/20 | 9/39/115/115  | -       |
| 25  | CLA  | k     | 614 | -    | -         | 11/23/99/115  | -       |
| 25  | CLA  | j     | 601 | 17   | 1/1/12/20 | 4/23/99/115   | -       |
| 25  | CLA  | m     | 605 | 17   | -         | 6/12/88/115   | -       |
| 35  | IHT  | a     | 317 | -    | -         | 10/25/65/65   | 0/2/2/2 |
| 32  | II0  | a     | 314 | -    | -         | 4/21/67/67    | 0/2/2/2 |
| 25  | CLA  | c     | 605 | 13   | 1/1/12/20 | 9/23/99/115   | -       |
| 25  | CLA  | A     | 815 | 37   | -         | 5/15/91/115   | -       |
| 25  | CLA  | A     | 824 | 37   | 1/1/15/20 | 10/39/115/115 | -       |
| 34  | KC2  | s     | 201 | 12   | -         | 9/15/71/71    | -       |
| 35  | IHT  | c     | 616 | -    | -         | 9/25/65/65    | 0/2/2/2 |
| 25  | CLA  | A     | 806 | -    | -         | 13/39/115/115 | -       |
| 35  | IHT  | j     | 616 | -    | -         | 7/25/65/65    | 0/2/2/2 |
| 32  | II0  | c     | 614 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 25  | CLA  | A     | 813 | -    | -         | 7/15/91/115   | -       |
| 32  | II0  | l     | 313 | -    | -         | 4/21/67/67    | 0/2/2/2 |
| 32  | II0  | n     | 319 | -    | -         | 6/21/67/67    | 0/2/2/2 |
| 32  | II0  | b     | 617 | -    | -         | 0/21/67/67    | 0/2/2/2 |
| 25  | CLA  | B     | 829 | -    | -         | 7/21/97/115   | -       |
| 30  | SF4  | C     | 102 | 3    | -         | -             | 0/6/5/5 |
| 25  | CLA  | a     | 304 | 14   | 1/1/12/20 | 6/21/97/115   | -       |
| 25  | CLA  | B     | 823 | 37   | -         | 13/38/114/115 | -       |
| 25  | CLA  | m     | 607 | -    | -         | 6/23/99/115   | -       |
| 35  | IHT  | k     | 618 | -    | -         | 10/25/65/65   | 0/2/2/2 |
| 34  | KC2  | j     | 610 | 17   | -         | 6/15/71/71    | -       |
| 25  | CLA  | j     | 606 | -    | 1/1/12/20 | 10/23/99/115  | -       |
| 25  | CLA  | d     | 301 | 21   | 1/1/12/20 | 2/21/97/115   | -       |
| 25  | CLA  | L     | 204 | -    | -         | 6/21/97/115   | -       |
| 25  | CLA  | A     | 835 | -    | 1/1/15/20 | 17/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27  | LHG  | d     | 317 | 25   | -         | 16/41/41/53   | -       |
| 35  | IHT  | n     | 318 | -    | -         | 8/25/65/65    | 0/2/2/2 |
| 32  | II0  | m     | 618 | -    | -         | 4/21/67/67    | 0/2/2/2 |
| 25  | CLA  | A     | 807 | 1    | 1/1/15/20 | 14/39/115/115 | -       |
| 32  | II0  | J     | 104 | -    | -         | 7/21/67/67    | 0/2/2/2 |
| 25  | CLA  | A     | 836 | -    | -         | 17/39/115/115 | -       |
| 25  | CLA  | l     | 304 | 18   | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | CLA  | L     | 203 | -    | -         | 13/39/115/115 | -       |
| 25  | CLA  | i     | 305 | 20   | -         | 13/39/115/115 | -       |
| 25  | CLA  | A     | 808 | 1    | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | CLA  | A     | 826 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 25  | CLA  | A     | 818 | -    | 1/1/15/20 | 21/39/115/115 | -       |
| 25  | CLA  | B     | 811 | -    | 1/1/13/20 | 10/27/103/115 | -       |
| 25  | CLA  | b     | 608 | 27   | 1/1/15/20 | 10/39/115/115 | -       |
| 25  | CLA  | k     | 602 | 19   | 1/1/12/20 | 7/21/97/115   | -       |
| 25  | CLA  | A     | 802 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 25  | CLA  | a     | 308 | 14   | 1/1/15/20 | 16/39/115/115 | -       |
| 25  | CLA  | n     | 305 | 23   | 1/1/14/20 | 10/33/109/115 | -       |
| 32  | II0  | d     | 314 | -    | -         | 3/21/67/67    | 0/2/2/2 |
| 28  | WVN  | h     | 309 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 25  | CLA  | n     | 302 | 23   | 1/1/11/20 | 6/15/91/115   | -       |
| 34  | KC2  | k     | 613 | 34   | -         | 11/15/71/71   | -       |
| 28  | WVN  | B     | 844 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 25  | CLA  | d     | 302 | -    | 1/1/12/20 | 7/23/99/115   | -       |
| 28  | WVN  | A     | 847 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 28  | WVN  | l     | 301 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 25  | CLA  | k     | 604 | -    | -         | 16/39/115/115 | -       |
| 28  | WVN  | L     | 206 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 25  | CLA  | n     | 304 | -    | 1/1/12/20 | 10/23/99/115  | -       |
| 28  | WVN  | J     | 102 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B     | 815 | -    | -         | 9/27/103/115  | -       |
| 34  | KC2  | d     | 311 | -    | -         | 6/15/71/71    | -       |
| 25  | CLA  | h     | 305 | 16   | 1/1/12/20 | 6/23/99/115   | -       |
| 25  | CLA  | A     | 816 | -    | -         | 18/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | Q     | 303 | 24   | 1/1/11/20 | 8/15/91/115   | -       |
| 25  | CLA  | h     | 303 | 16   | 1/1/12/20 | 9/21/97/115   | -       |
| 29  | LMT  | a     | 302 | -    | -         | 4/15/35/61    | 0/1/1/2 |
| 25  | CLA  | B     | 826 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 32  | II0  | l     | 314 | -    | -         | 7/21/67/67    | 0/2/2/2 |
| 32  | II0  | a     | 316 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 25  | CLA  | A     | 811 | -    | -         | 9/26/102/115  | -       |
| 25  | CLA  | A     | 834 | -    | 1/1/12/20 | 6/23/99/115   | -       |
| 25  | CLA  | m     | 610 | 27   | 1/1/13/20 | 13/27/103/115 | -       |
| 25  | CLA  | A     | 841 | -    | 1/1/15/20 | 20/39/115/115 | -       |
| 25  | CLA  | j     | 602 | 17   | -         | 6/21/97/115   | -       |
| 25  | CLA  | B     | 830 | 37   | -         | 18/39/115/115 | -       |
| 27  | LHG  | J     | 107 | -    | -         | 8/35/35/53    | -       |
| 25  | CLA  | A     | 838 | 27   | 1/1/12/20 | 6/24/100/115  | -       |
| 25  | CLA  | s     | 209 | -    | 1/1/12/20 | 7/23/99/115   | -       |
| 25  | CLA  | n     | 308 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 28  | WVN  | F     | 203 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 25  | CLA  | c     | 609 | 27   | 1/1/11/20 | 7/15/91/115   | -       |
| 29  | LMT  | b     | 618 | -    | -         | 9/15/35/61    | 0/1/1/2 |
| 25  | CLA  | c     | 611 | -    | -         | 10/15/91/115  | -       |
| 29  | LMT  | A     | 852 | -    | -         | 13/21/61/61   | 0/2/2/2 |
| 35  | IHT  | b     | 616 | -    | -         | 6/25/65/65    | 0/2/2/2 |
| 28  | WVN  | B     | 849 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 34  | KC2  | n     | 312 | 23   | -         | 4/15/71/71    | -       |
| 25  | CLA  | a     | 309 | 14   | 1/1/15/20 | 9/39/115/115  | -       |
| 25  | CLA  | B     | 814 | -    | 1/1/13/20 | 12/32/108/115 | -       |
| 25  | CLA  | m     | 608 | 17   | 1/1/15/20 | 15/39/115/115 | -       |
| 32  | II0  | k     | 619 | -    | -         | 6/21/67/67    | 0/2/2/2 |

The worst 5 of 3400 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 35  | R     | 203 | IHT  | C15-C11 | 25.30 | 1.63        | 1.35     |
| 35  | b     | 616 | IHT  | C15-C11 | 25.26 | 1.63        | 1.35     |
| 35  | a     | 317 | IHT  | C15-C11 | 25.12 | 1.62        | 1.35     |
| 35  | k     | 618 | IHT  | C15-C11 | 24.95 | 1.62        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 35  | n     | 318 | IHT  | C15-C11 | 24.93 | 1.62        | 1.35     |

The worst 5 of 3717 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 34  | m     | 611 | KC2  | C1A-NA-C4A | -12.55 | 100.95      | 106.68   |
| 34  | j     | 610 | KC2  | C1A-NA-C4A | -12.38 | 101.03      | 106.68   |
| 34  | s     | 204 | KC2  | C1A-NA-C4A | -12.13 | 101.15      | 106.68   |
| 34  | l     | 311 | KC2  | C1A-NA-C4A | -11.90 | 101.25      | 106.68   |
| 34  | n     | 312 | KC2  | C1A-NA-C4A | -11.86 | 101.27      | 106.68   |

5 of 161 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25  | A     | 801 | CLA  | ND   |
| 25  | A     | 802 | CLA  | ND   |
| 25  | A     | 804 | CLA  | ND   |
| 25  | A     | 805 | CLA  | ND   |
| 25  | A     | 807 | CLA  | ND   |

5 of 3463 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | A     | 801 | CLA  | CBD-CGD-O2D-CED |
| 25  | A     | 802 | CLA  | CBA-CGA-O2A-C1  |
| 25  | A     | 802 | CLA  | O1A-CGA-O2A-C1  |
| 25  | A     | 803 | CLA  | C1A-C2A-CAA-CBA |
| 25  | A     | 803 | CLA  | C3A-C2A-CAA-CBA |

There are no ring outliers.

231 monomers are involved in 541 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 32  | d     | 315 | II0  | 1       | 0            |
| 25  | A     | 853 | CLA  | 2       | 0            |
| 25  | K     | 102 | CLA  | 1       | 0            |
| 25  | l     | 309 | CLA  | 1       | 0            |
| 25  | F     | 201 | CLA  | 2       | 0            |
| 25  | d     | 306 | CLA  | 2       | 0            |
| 25  | A     | 805 | CLA  | 1       | 0            |
| 28  | J     | 101 | WVN  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | J     | 103 | CLA  | 3       | 0            |
| 36  | i     | 301 | LMU  | 2       | 0            |
| 25  | B     | 804 | CLA  | 5       | 0            |
| 25  | A     | 825 | CLA  | 2       | 0            |
| 25  | A     | 854 | CLA  | 5       | 0            |
| 25  | j     | 607 | CLA  | 1       | 0            |
| 25  | B     | 835 | CLA  | 6       | 0            |
| 25  | c     | 606 | CLA  | 3       | 0            |
| 25  | n     | 307 | CLA  | 2       | 0            |
| 33  | J     | 105 | LMG  | 1       | 0            |
| 25  | d     | 303 | CLA  | 4       | 0            |
| 25  | B     | 837 | CLA  | 11      | 0            |
| 25  | B     | 806 | CLA  | 13      | 0            |
| 25  | l     | 306 | CLA  | 5       | 0            |
| 25  | k     | 605 | CLA  | 2       | 0            |
| 25  | B     | 820 | CLA  | 1       | 0            |
| 32  | n     | 301 | II0  | 1       | 0            |
| 25  | c     | 604 | CLA  | 3       | 0            |
| 27  | m     | 617 | LHG  | 2       | 0            |
| 30  | B     | 802 | SF4  | 7       | 0            |
| 25  | b     | 609 | CLA  | 2       | 0            |
| 28  | M     | 101 | WVN  | 3       | 0            |
| 25  | A     | 803 | CLA  | 3       | 0            |
| 25  | s     | 202 | CLA  | 3       | 0            |
| 25  | b     | 601 | CLA  | 2       | 0            |
| 25  | A     | 833 | CLA  | 1       | 0            |
| 27  | A     | 845 | LHG  | 1       | 0            |
| 25  | d     | 307 | CLA  | 1       | 0            |
| 25  | c     | 608 | CLA  | 2       | 0            |
| 25  | b     | 602 | CLA  | 2       | 0            |
| 25  | n     | 311 | CLA  | 4       | 0            |
| 25  | B     | 850 | CLA  | 3       | 0            |
| 25  | k     | 607 | CLA  | 2       | 0            |
| 25  | m     | 601 | CLA  | 1       | 0            |
| 25  | B     | 803 | CLA  | 3       | 0            |
| 25  | A     | 812 | CLA  | 6       | 0            |
| 25  | m     | 606 | CLA  | 1       | 0            |
| 25  | A     | 855 | CLA  | 6       | 0            |
| 34  | k     | 612 | KC2  | 2       | 0            |
| 25  | i     | 302 | CLA  | 1       | 0            |
| 25  | A     | 819 | CLA  | 2       | 0            |
| 25  | n     | 309 | CLA  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | a     | 310 | CLA  | 1       | 0            |
| 25  | A     | 843 | CLA  | 8       | 0            |
| 25  | B     | 810 | CLA  | 4       | 0            |
| 25  | l     | 305 | CLA  | 1       | 0            |
| 35  | b     | 615 | IHT  | 1       | 0            |
| 27  | L     | 207 | LHG  | 3       | 0            |
| 25  | c     | 612 | CLA  | 3       | 0            |
| 25  | j     | 609 | CLA  | 4       | 0            |
| 25  | h     | 307 | CLA  | 2       | 0            |
| 25  | k     | 608 | CLA  | 5       | 0            |
| 25  | c     | 607 | CLA  | 1       | 0            |
| 25  | b     | 605 | CLA  | 2       | 0            |
| 25  | k     | 606 | CLA  | 1       | 0            |
| 25  | h     | 301 | CLA  | 3       | 0            |
| 35  | m     | 616 | IHT  | 1       | 0            |
| 25  | B     | 808 | CLA  | 6       | 0            |
| 25  | A     | 840 | CLA  | 3       | 0            |
| 25  | B     | 833 | CLA  | 6       | 0            |
| 25  | A     | 822 | CLA  | 1       | 0            |
| 25  | m     | 603 | CLA  | 4       | 0            |
| 32  | j     | 613 | II0  | 1       | 0            |
| 25  | j     | 612 | CLA  | 4       | 0            |
| 25  | i     | 309 | CLA  | 1       | 0            |
| 25  | B     | 812 | CLA  | 4       | 0            |
| 27  | B     | 801 | LHG  | 5       | 0            |
| 33  | n     | 321 | LMG  | 5       | 0            |
| 25  | n     | 310 | CLA  | 1       | 0            |
| 27  | a     | 319 | LHG  | 1       | 0            |
| 25  | a     | 311 | CLA  | 2       | 0            |
| 25  | A     | 837 | CLA  | 5       | 0            |
| 32  | i     | 313 | II0  | 1       | 0            |
| 25  | B     | 825 | CLA  | 3       | 0            |
| 25  | i     | 312 | CLA  | 2       | 0            |
| 26  | A     | 844 | PQN  | 10      | 0            |
| 25  | B     | 816 | CLA  | 6       | 0            |
| 25  | B     | 824 | CLA  | 3       | 0            |
| 25  | l     | 312 | CLA  | 1       | 0            |
| 25  | B     | 805 | CLA  | 6       | 0            |
| 25  | h     | 308 | CLA  | 3       | 0            |
| 25  | c     | 602 | CLA  | 3       | 0            |
| 25  | k     | 603 | CLA  | 1       | 0            |
| 25  | B     | 809 | CLA  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | d     | 305 | CLA  | 1       | 0            |
| 25  | m     | 602 | CLA  | 1       | 0            |
| 25  | A     | 827 | CLA  | 2       | 0            |
| 25  | B     | 821 | CLA  | 3       | 0            |
| 25  | j     | 605 | CLA  | 1       | 0            |
| 31  | B     | 843 | DGD  | 7       | 0            |
| 25  | b     | 606 | CLA  | 3       | 0            |
| 25  | K     | 101 | CLA  | 2       | 0            |
| 25  | A     | 832 | CLA  | 3       | 0            |
| 26  | B     | 842 | PQN  | 2       | 0            |
| 25  | b     | 610 | CLA  | 4       | 0            |
| 25  | a     | 303 | CLA  | 2       | 0            |
| 25  | A     | 817 | CLA  | 2       | 0            |
| 25  | A     | 810 | CLA  | 1       | 0            |
| 25  | i     | 304 | CLA  | 2       | 0            |
| 33  | Q     | 301 | LMG  | 1       | 0            |
| 25  | A     | 809 | CLA  | 2       | 0            |
| 27  | b     | 619 | LHG  | 2       | 0            |
| 33  | c     | 619 | LMG  | 5       | 0            |
| 25  | d     | 308 | CLA  | 1       | 0            |
| 25  | B     | 807 | CLA  | 5       | 0            |
| 25  | b     | 612 | CLA  | 4       | 0            |
| 25  | k     | 609 | CLA  | 5       | 0            |
| 25  | j     | 608 | CLA  | 1       | 0            |
| 27  | i     | 318 | LHG  | 2       | 0            |
| 25  | B     | 832 | CLA  | 4       | 0            |
| 25  | B     | 818 | CLA  | 2       | 0            |
| 25  | m     | 612 | CLA  | 1       | 0            |
| 25  | i     | 308 | CLA  | 4       | 0            |
| 25  | B     | 839 | CLA  | 3       | 0            |
| 25  | j     | 604 | CLA  | 2       | 0            |
| 25  | n     | 306 | CLA  | 1       | 0            |
| 25  | s     | 203 | CLA  | 4       | 0            |
| 25  | B     | 834 | CLA  | 2       | 0            |
| 25  | s     | 206 | CLA  | 1       | 0            |
| 25  | B     | 817 | CLA  | 1       | 0            |
| 34  | i     | 319 | KC2  | 5       | 0            |
| 32  | c     | 615 | II0  | 1       | 0            |
| 25  | b     | 611 | CLA  | 4       | 0            |
| 25  | A     | 823 | CLA  | 5       | 0            |
| 27  | k     | 620 | LHG  | 1       | 0            |
| 27  | l     | 317 | LHG  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | B     | 841 | CLA  | 3       | 0            |
| 25  | B     | 838 | CLA  | 6       | 0            |
| 25  | A     | 821 | CLA  | 1       | 0            |
| 25  | n     | 303 | CLA  | 2       | 0            |
| 25  | A     | 842 | CLA  | 5       | 0            |
| 27  | a     | 301 | LHG  | 2       | 0            |
| 27  | J     | 106 | LHG  | 6       | 0            |
| 25  | A     | 814 | CLA  | 2       | 0            |
| 33  | b     | 620 | LMG  | 2       | 0            |
| 25  | B     | 822 | CLA  | 6       | 0            |
| 27  | c     | 620 | LHG  | 3       | 0            |
| 28  | B     | 846 | WVN  | 1       | 0            |
| 25  | m     | 613 | CLA  | 1       | 0            |
| 25  | h     | 306 | CLA  | 5       | 0            |
| 25  | A     | 830 | CLA  | 3       | 0            |
| 25  | a     | 312 | CLA  | 4       | 0            |
| 25  | i     | 311 | CLA  | 4       | 0            |
| 28  | s     | 205 | WVN  | 1       | 0            |
| 25  | h     | 302 | CLA  | 1       | 0            |
| 25  | A     | 828 | CLA  | 1       | 0            |
| 27  | n     | 320 | LHG  | 1       | 0            |
| 25  | l     | 307 | CLA  | 4       | 0            |
| 25  | R     | 202 | CLA  | 2       | 0            |
| 25  | A     | 829 | CLA  | 1       | 0            |
| 25  | A     | 856 | CLA  | 2       | 0            |
| 25  | B     | 840 | CLA  | 3       | 0            |
| 25  | A     | 804 | CLA  | 6       | 0            |
| 33  | s     | 208 | LMG  | 4       | 0            |
| 25  | i     | 303 | CLA  | 2       | 0            |
| 25  | B     | 828 | CLA  | 1       | 0            |
| 25  | b     | 603 | CLA  | 1       | 0            |
| 25  | B     | 827 | CLA  | 3       | 0            |
| 25  | A     | 839 | CLA  | 8       | 0            |
| 25  | h     | 313 | CLA  | 1       | 0            |
| 25  | A     | 831 | CLA  | 3       | 0            |
| 25  | B     | 813 | CLA  | 3       | 0            |
| 25  | A     | 801 | CLA  | 4       | 0            |
| 25  | L     | 202 | CLA  | 2       | 0            |
| 25  | k     | 601 | CLA  | 3       | 0            |
| 25  | A     | 820 | CLA  | 3       | 0            |
| 25  | Q     | 302 | CLA  | 4       | 0            |
| 25  | m     | 604 | CLA  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | j     | 603 | CLA  | 1       | 0            |
| 25  | b     | 604 | CLA  | 3       | 0            |
| 30  | C     | 101 | SF4  | 1       | 0            |
| 25  | B     | 836 | CLA  | 4       | 0            |
| 25  | l     | 308 | CLA  | 3       | 0            |
| 25  | k     | 614 | CLA  | 2       | 0            |
| 25  | j     | 601 | CLA  | 1       | 0            |
| 25  | A     | 824 | CLA  | 2       | 0            |
| 25  | A     | 806 | CLA  | 4       | 0            |
| 35  | j     | 616 | IHT  | 1       | 0            |
| 32  | c     | 614 | II0  | 1       | 0            |
| 30  | C     | 102 | SF4  | 5       | 0            |
| 25  | B     | 823 | CLA  | 1       | 0            |
| 25  | m     | 607 | CLA  | 1       | 0            |
| 35  | k     | 618 | IHT  | 1       | 0            |
| 25  | d     | 301 | CLA  | 1       | 0            |
| 25  | L     | 204 | CLA  | 2       | 0            |
| 25  | A     | 835 | CLA  | 3       | 0            |
| 35  | n     | 318 | IHT  | 1       | 0            |
| 25  | A     | 807 | CLA  | 2       | 0            |
| 25  | A     | 836 | CLA  | 5       | 0            |
| 25  | l     | 304 | CLA  | 3       | 0            |
| 25  | L     | 203 | CLA  | 5       | 0            |
| 25  | i     | 305 | CLA  | 3       | 0            |
| 25  | A     | 808 | CLA  | 1       | 0            |
| 25  | A     | 826 | CLA  | 5       | 0            |
| 25  | A     | 818 | CLA  | 7       | 0            |
| 25  | b     | 608 | CLA  | 2       | 0            |
| 25  | k     | 602 | CLA  | 2       | 0            |
| 25  | A     | 802 | CLA  | 8       | 0            |
| 25  | a     | 308 | CLA  | 3       | 0            |
| 25  | n     | 305 | CLA  | 4       | 0            |
| 25  | n     | 302 | CLA  | 4       | 0            |
| 34  | k     | 613 | KC2  | 1       | 0            |
| 25  | d     | 302 | CLA  | 2       | 0            |
| 25  | k     | 604 | CLA  | 1       | 0            |
| 25  | n     | 304 | CLA  | 2       | 0            |
| 25  | B     | 815 | CLA  | 1       | 0            |
| 25  | A     | 816 | CLA  | 1       | 0            |
| 29  | a     | 302 | LMT  | 1       | 0            |
| 25  | B     | 826 | CLA  | 3       | 0            |
| 25  | A     | 834 | CLA  | 1       | 0            |

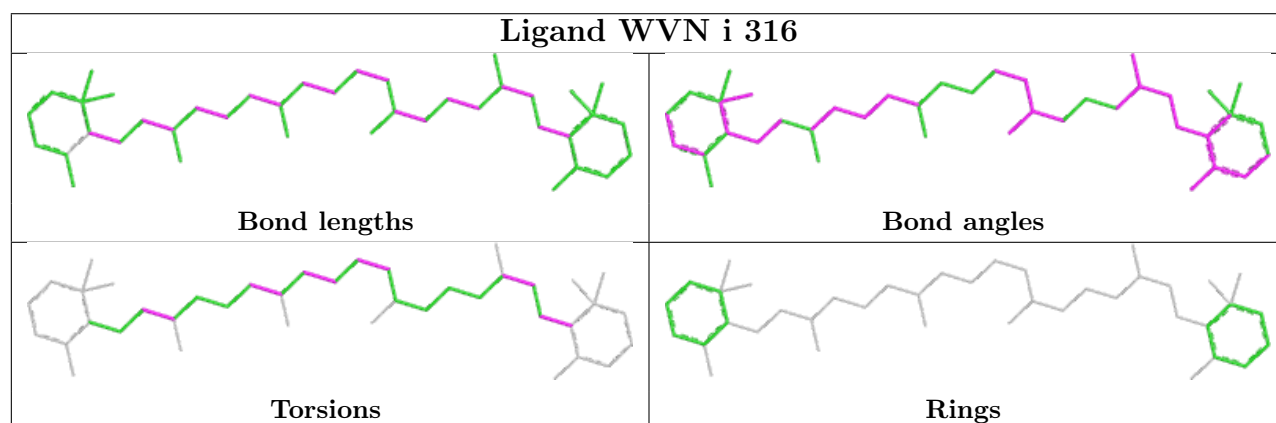
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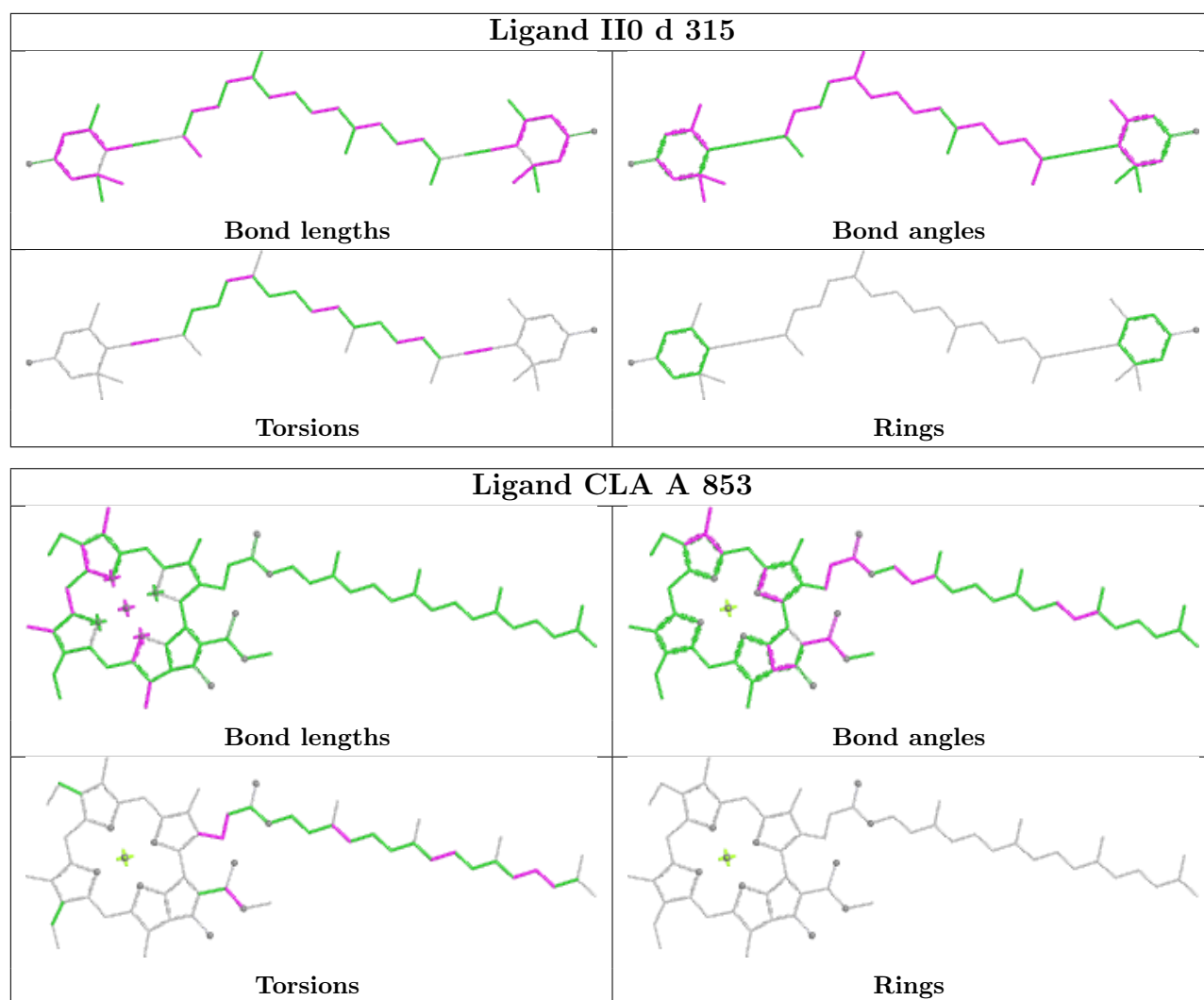


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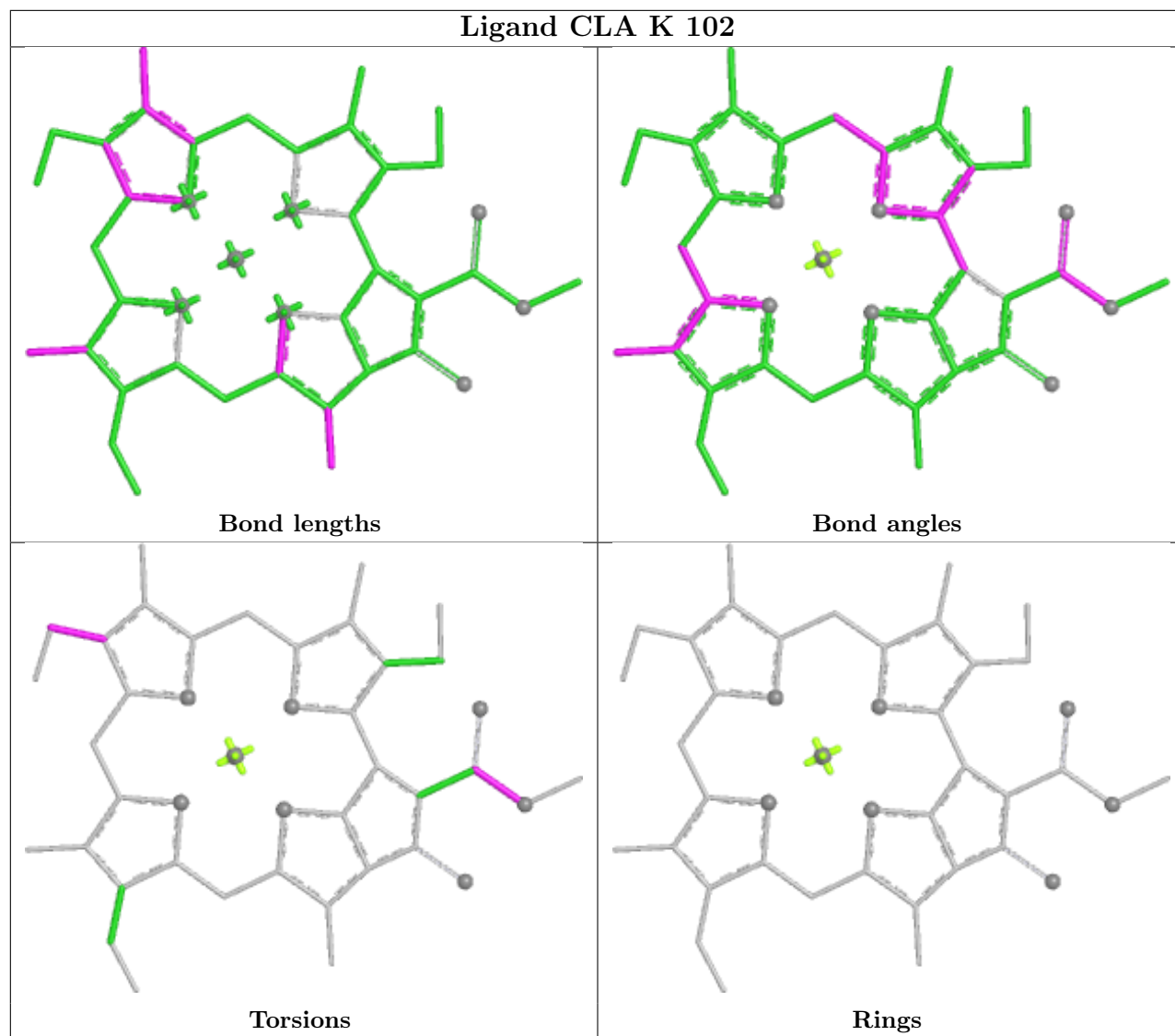
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | m     | 610 | CLA  | 3       | 0            |
| 25  | A     | 841 | CLA  | 7       | 0            |
| 25  | B     | 830 | CLA  | 3       | 0            |
| 27  | J     | 107 | LHG  | 2       | 0            |
| 25  | A     | 838 | CLA  | 1       | 0            |
| 25  | s     | 209 | CLA  | 2       | 0            |
| 25  | n     | 308 | CLA  | 2       | 0            |
| 28  | F     | 203 | WVN  | 1       | 0            |
| 29  | b     | 618 | LMT  | 3       | 0            |
| 25  | c     | 611 | CLA  | 2       | 0            |
| 29  | A     | 852 | LMT  | 2       | 0            |
| 25  | B     | 814 | CLA  | 2       | 0            |
| 25  | m     | 608 | CLA  | 3       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

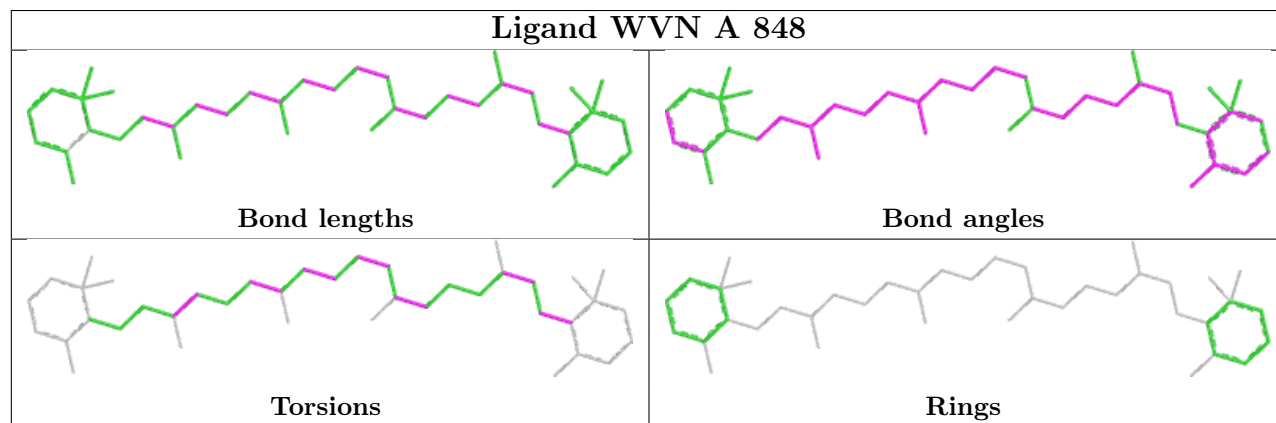


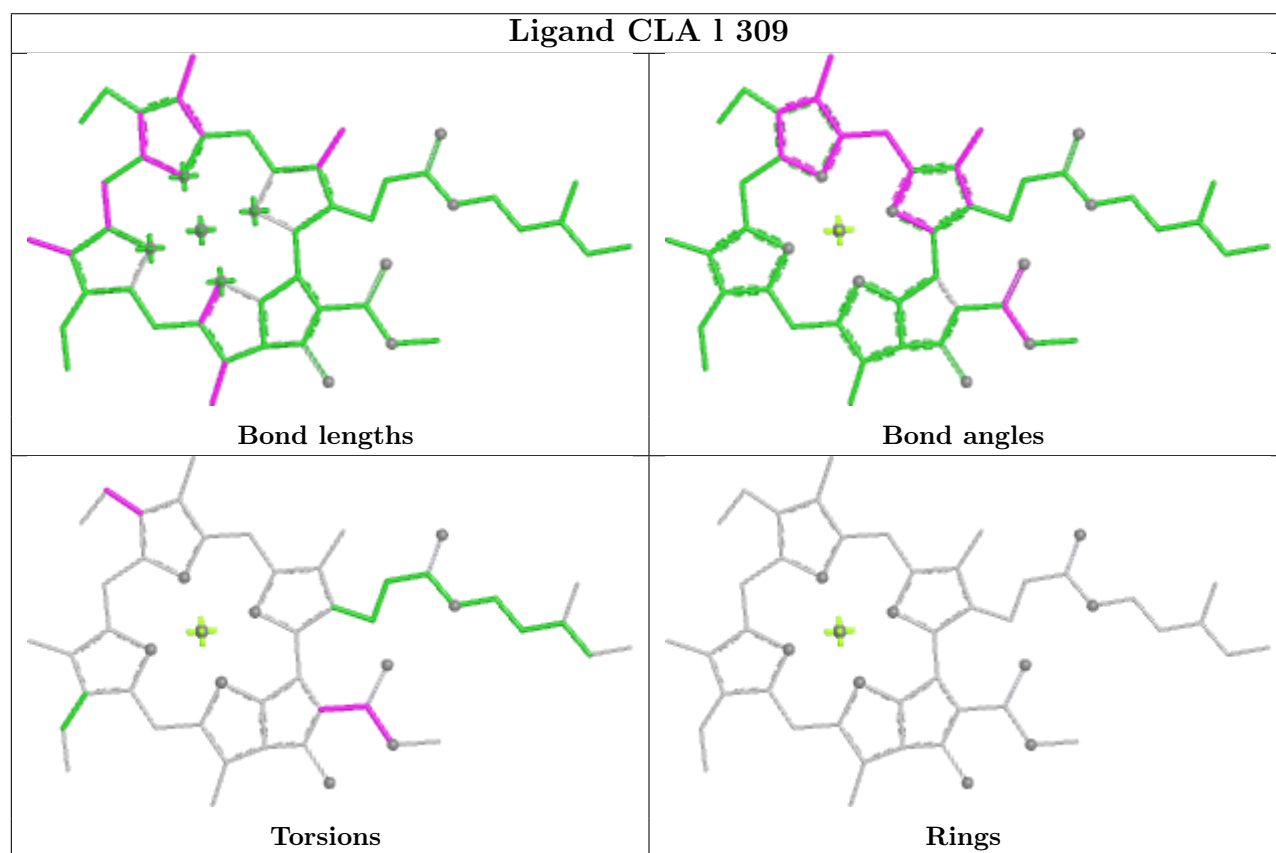
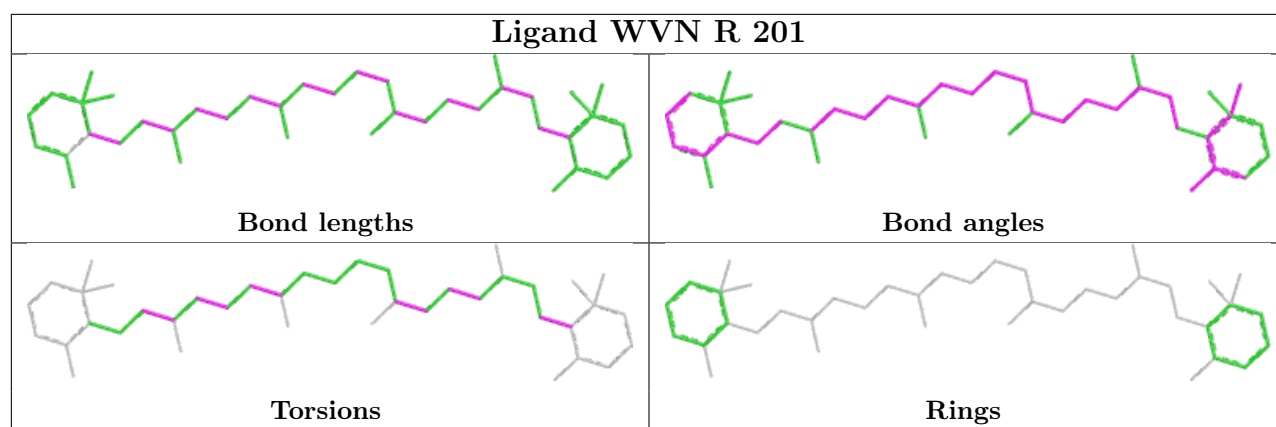


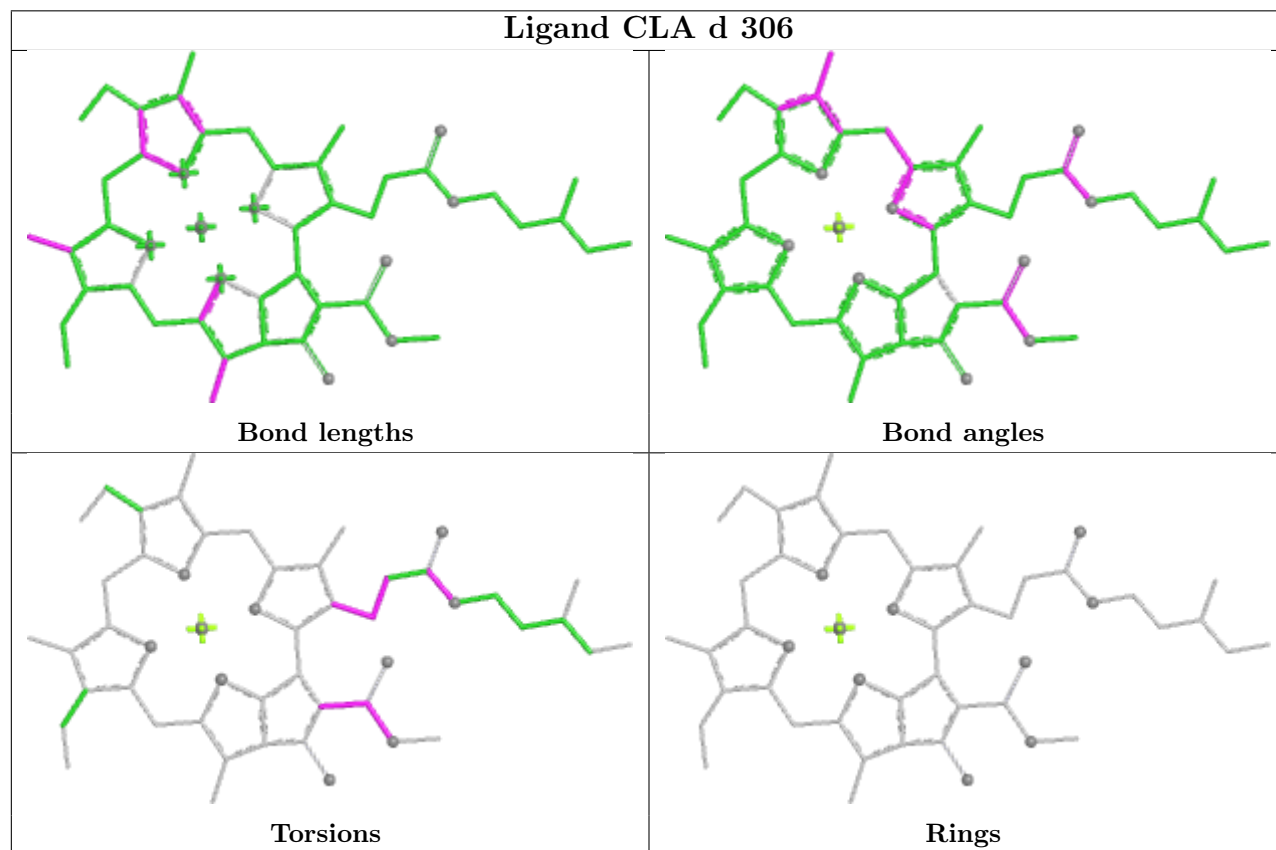
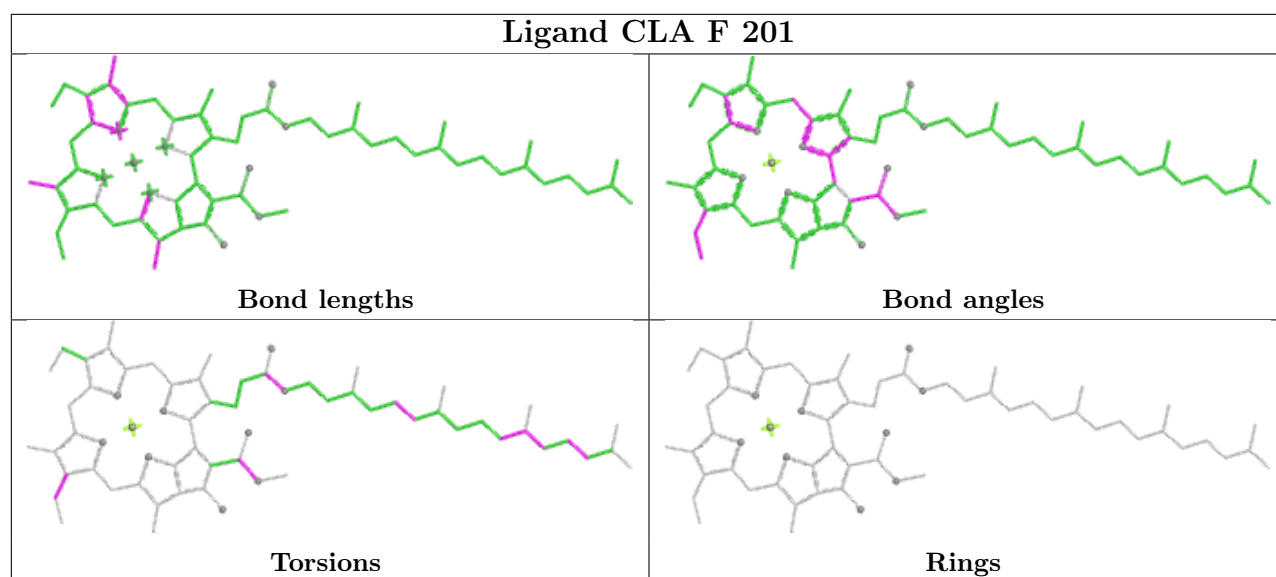
## Ligand CLA K 102

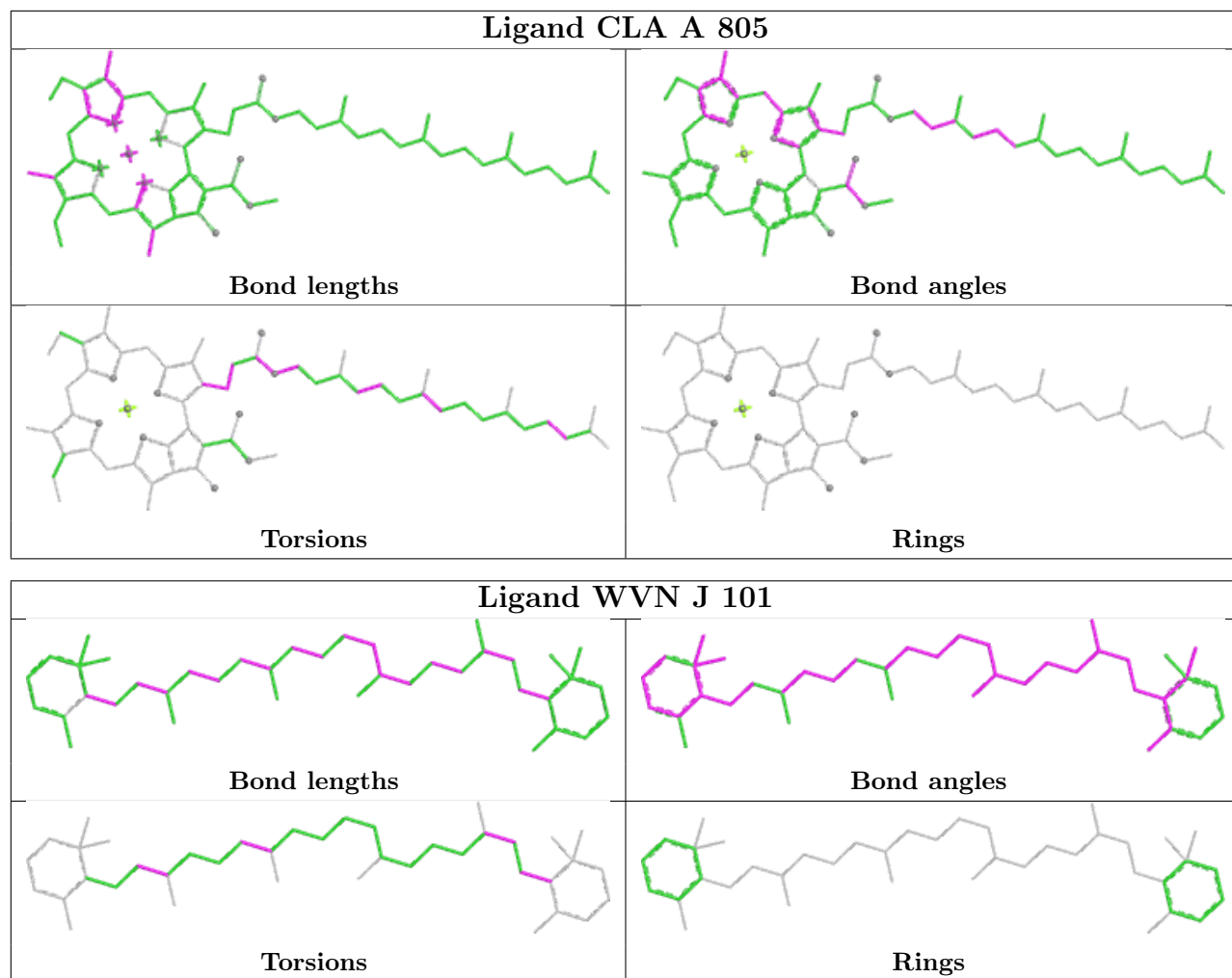


## Ligand WVN A 848

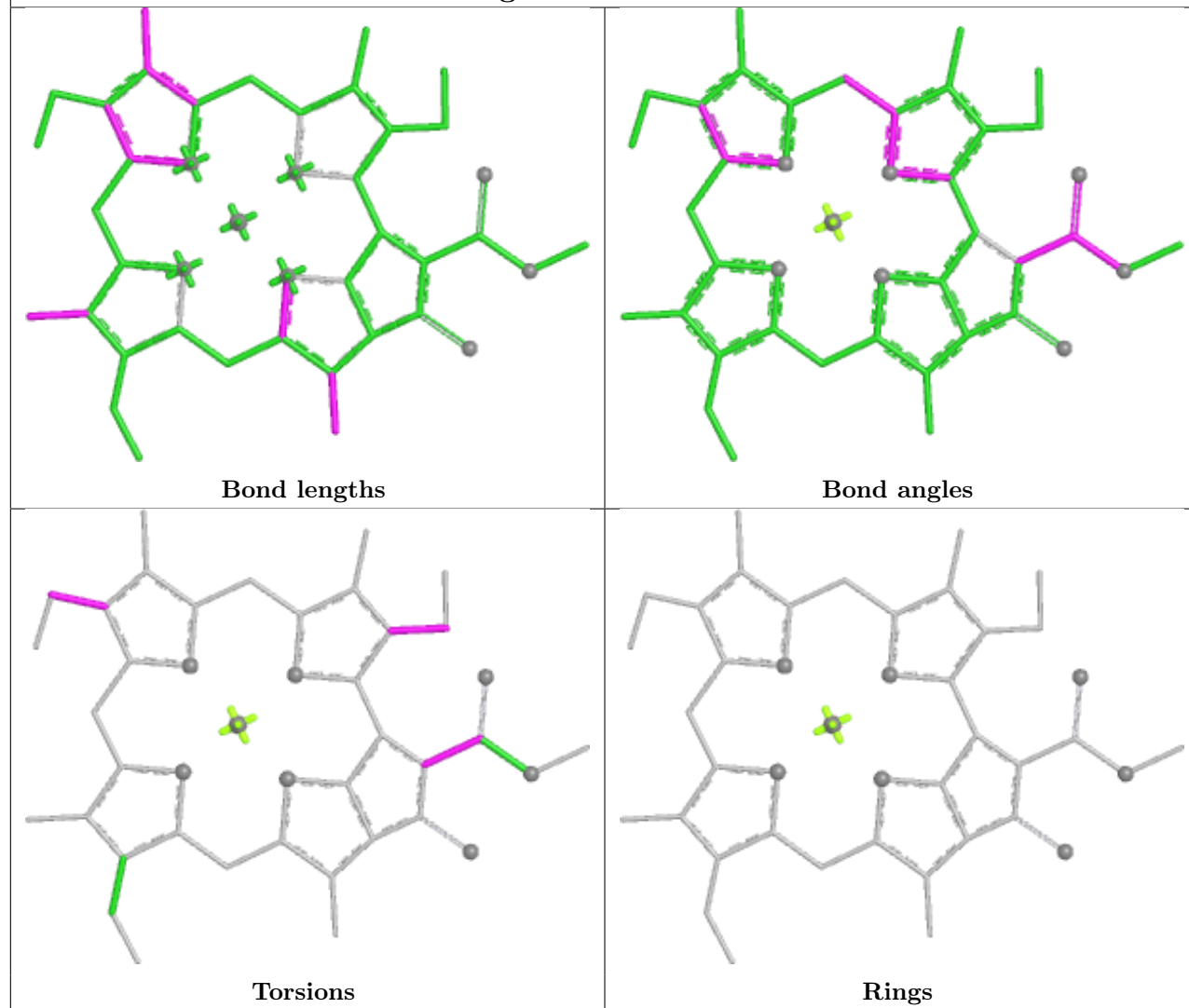




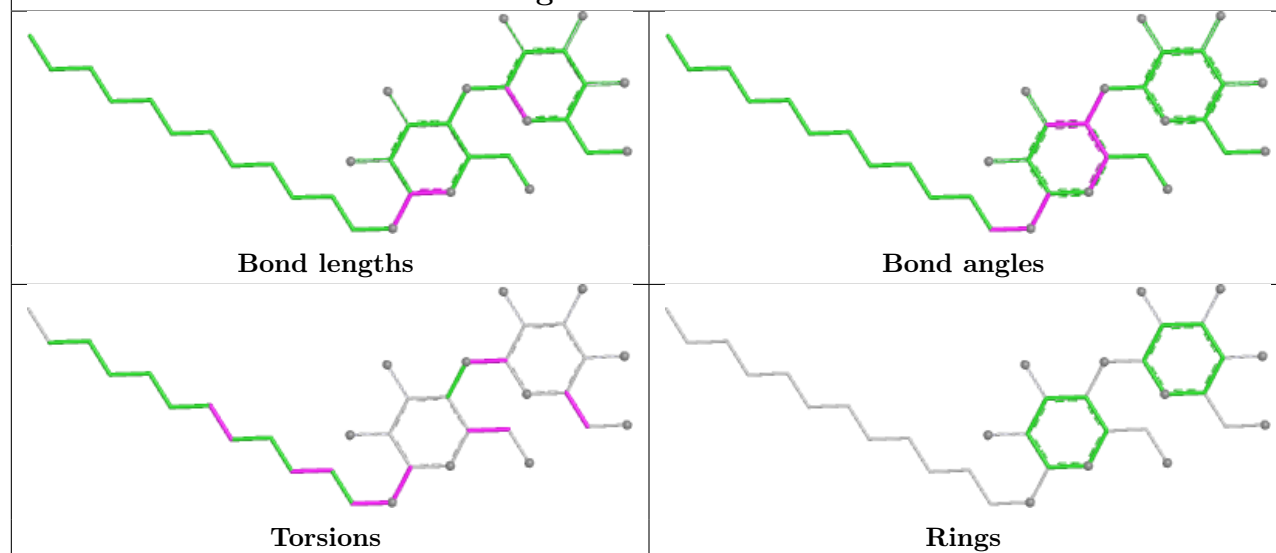


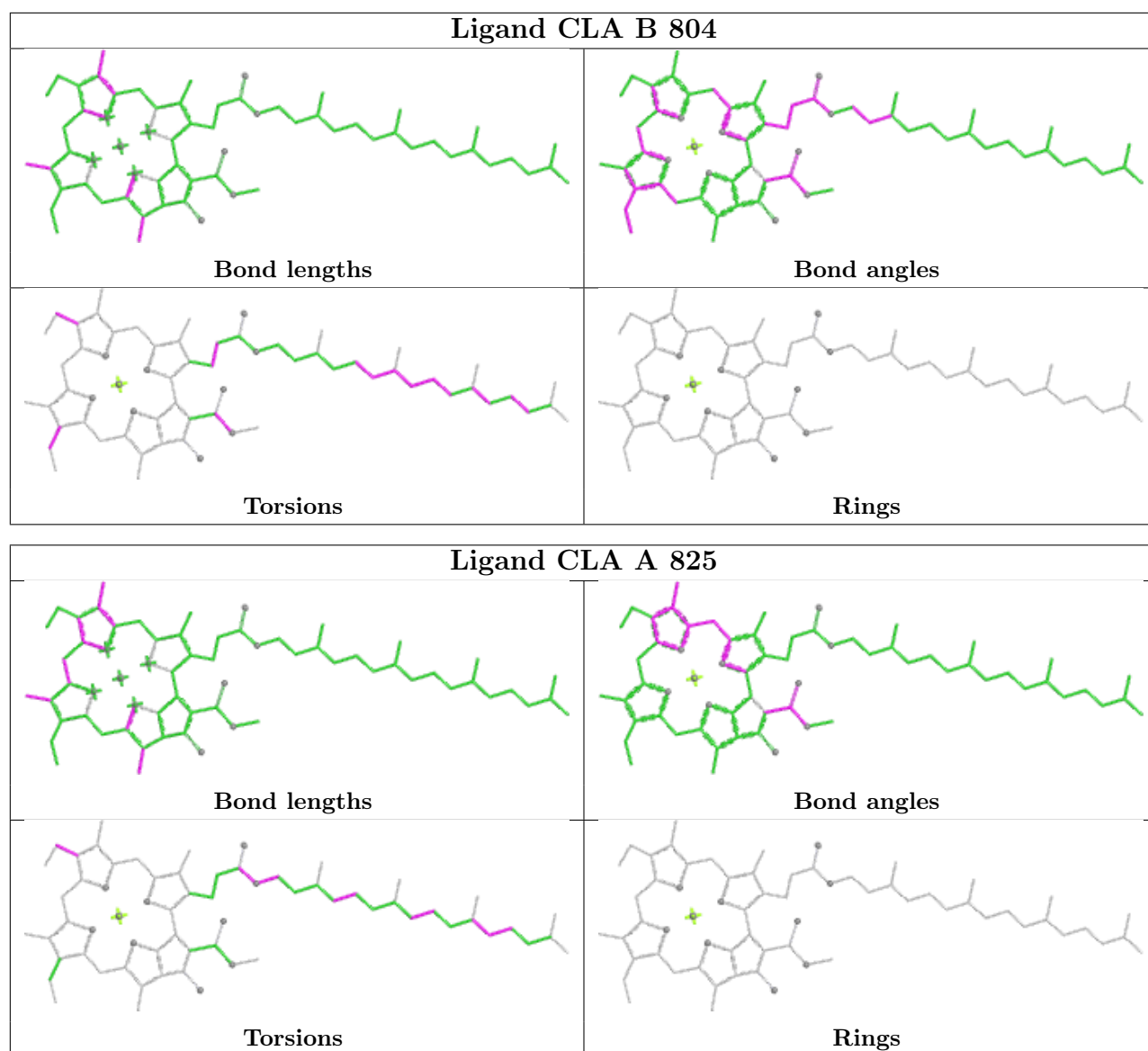


## Ligand CLA J 103



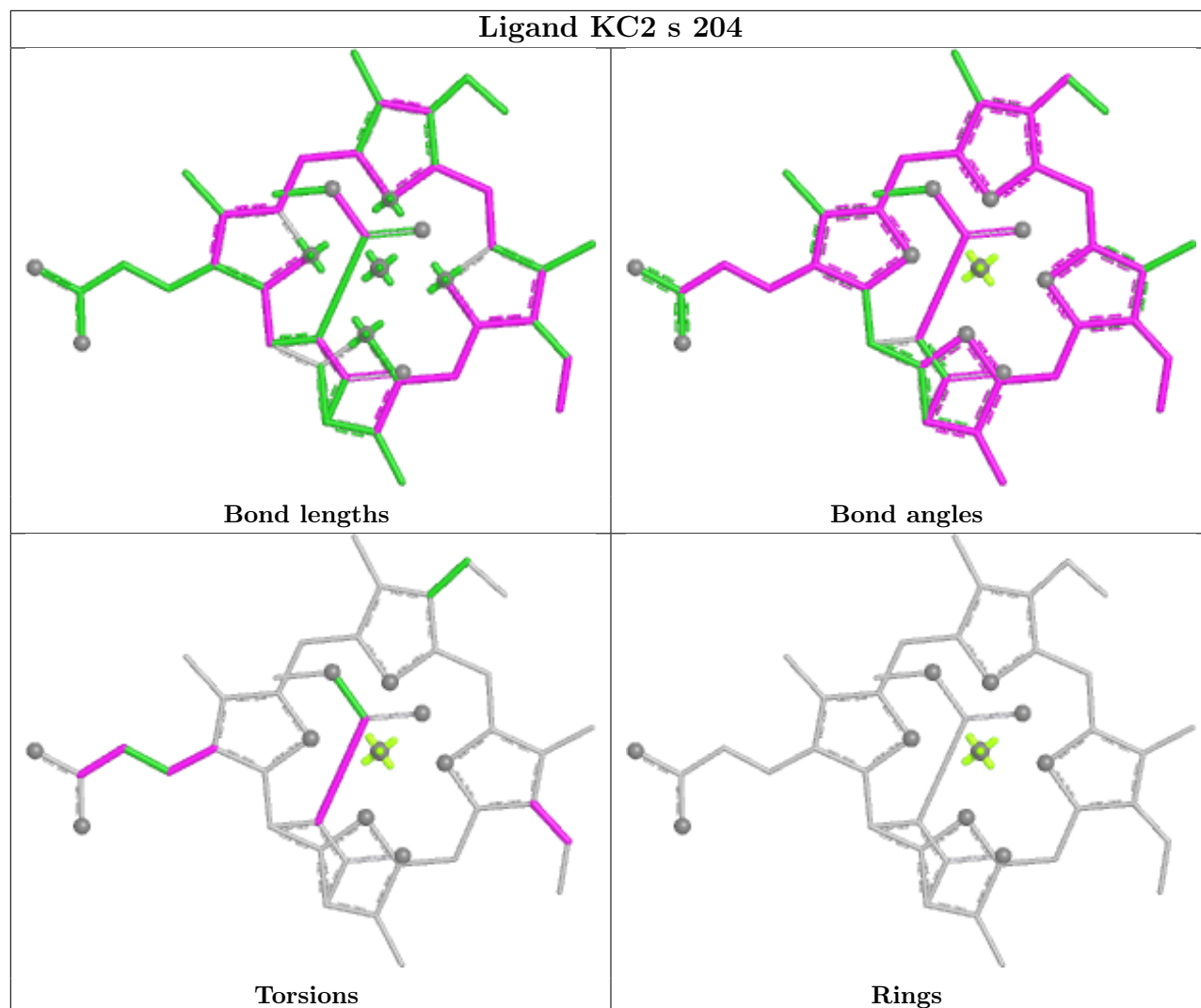
## Ligand LMU i 301



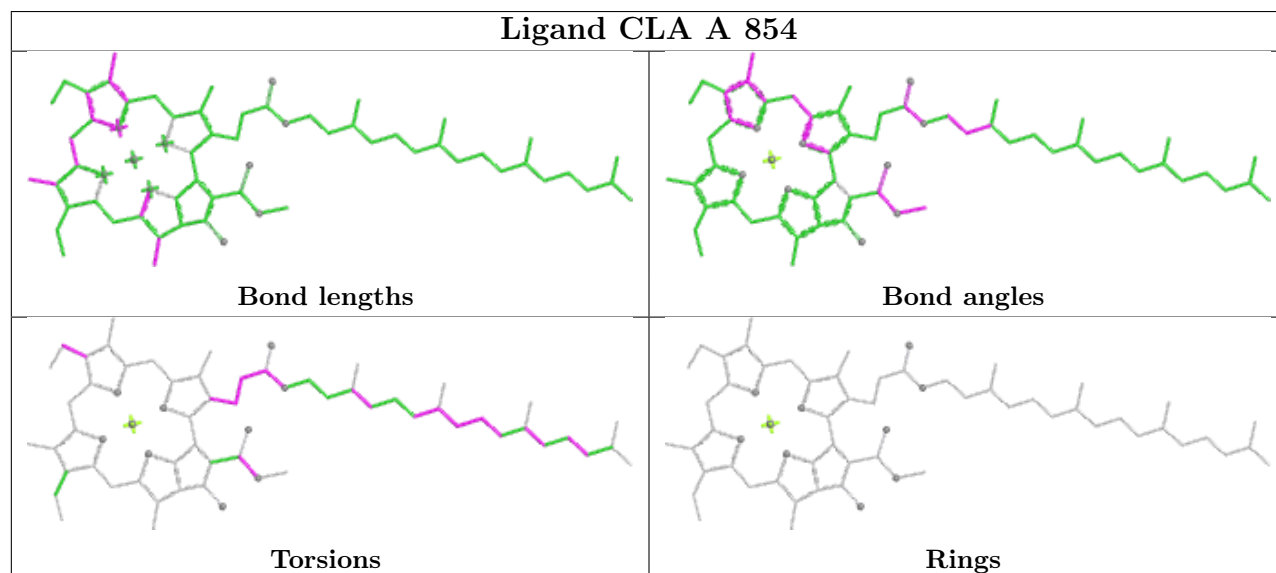


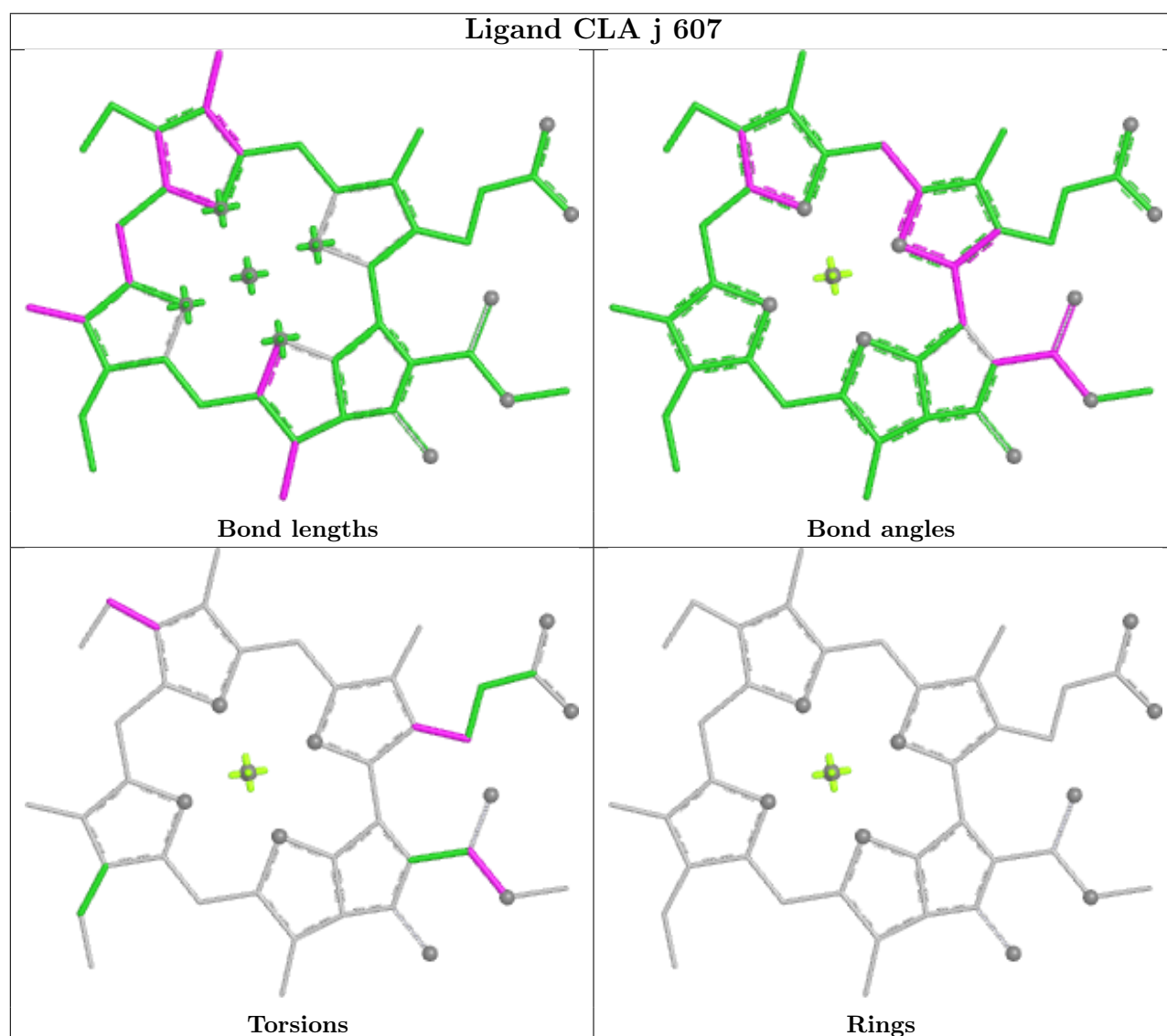
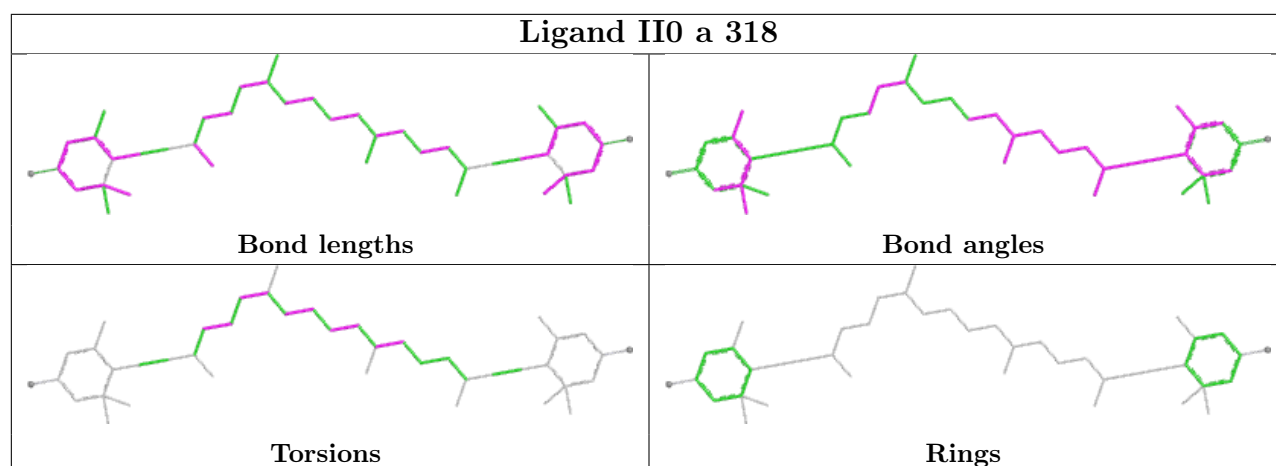


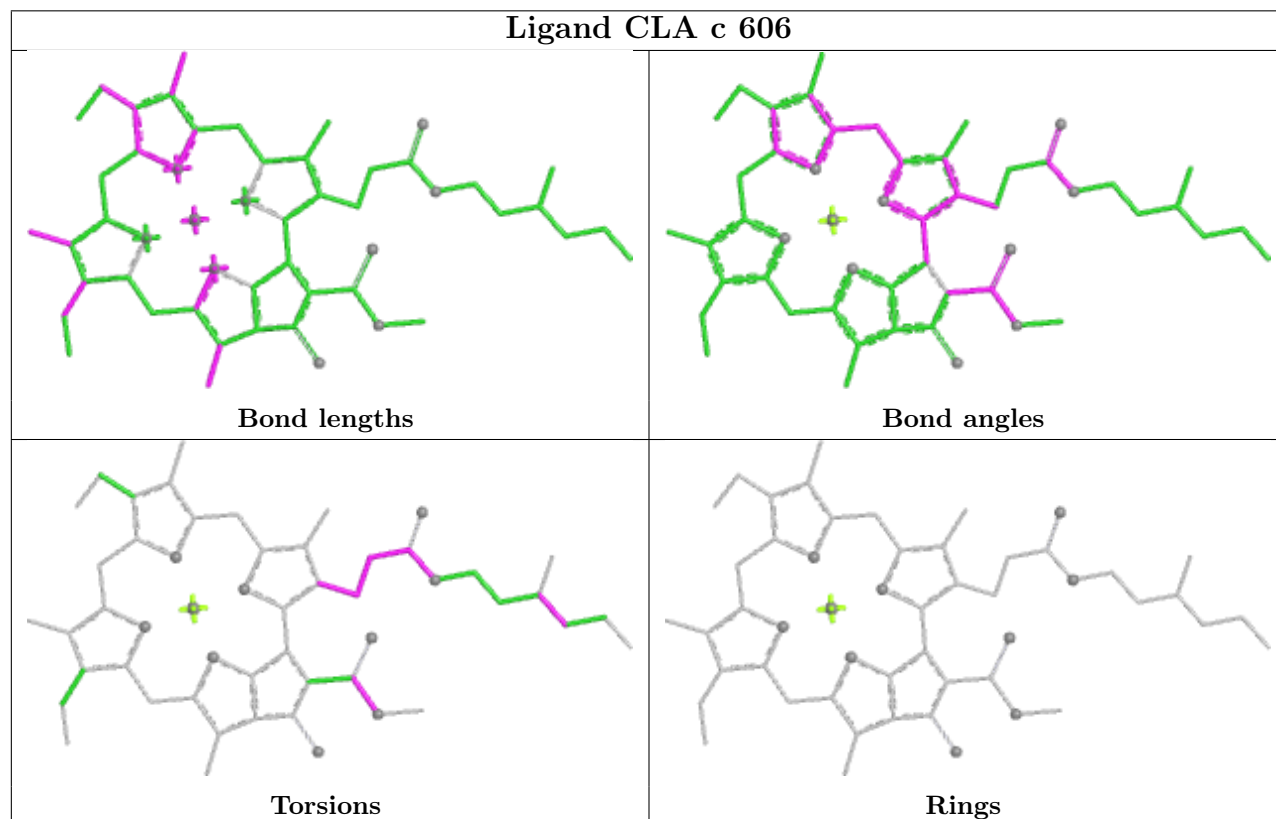
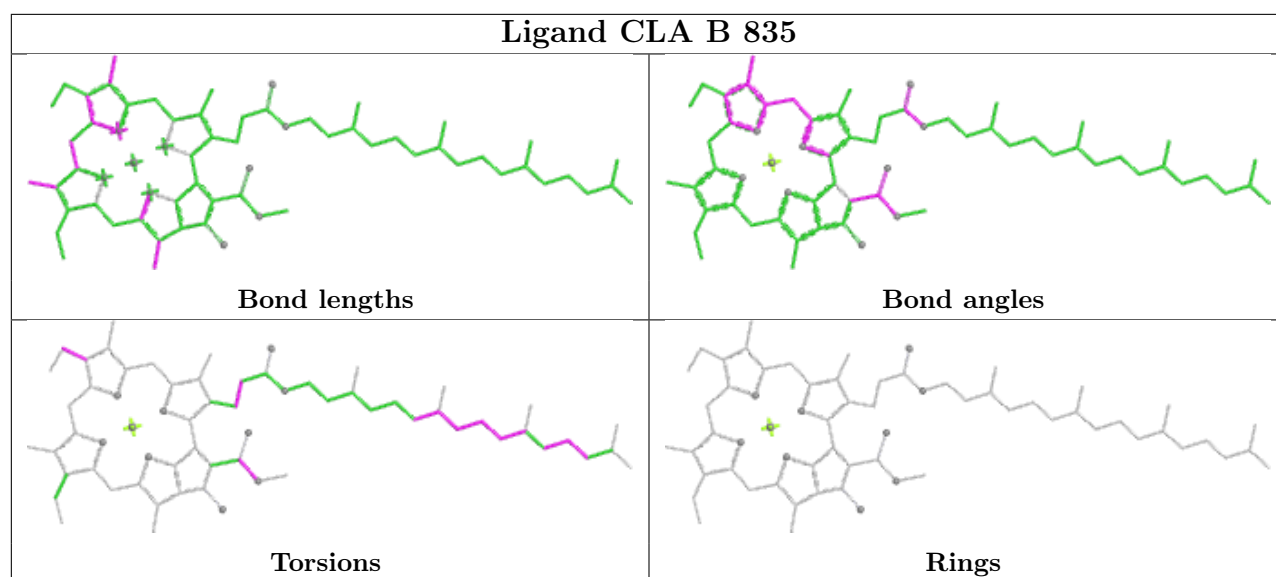
## Ligand KC2 s 204



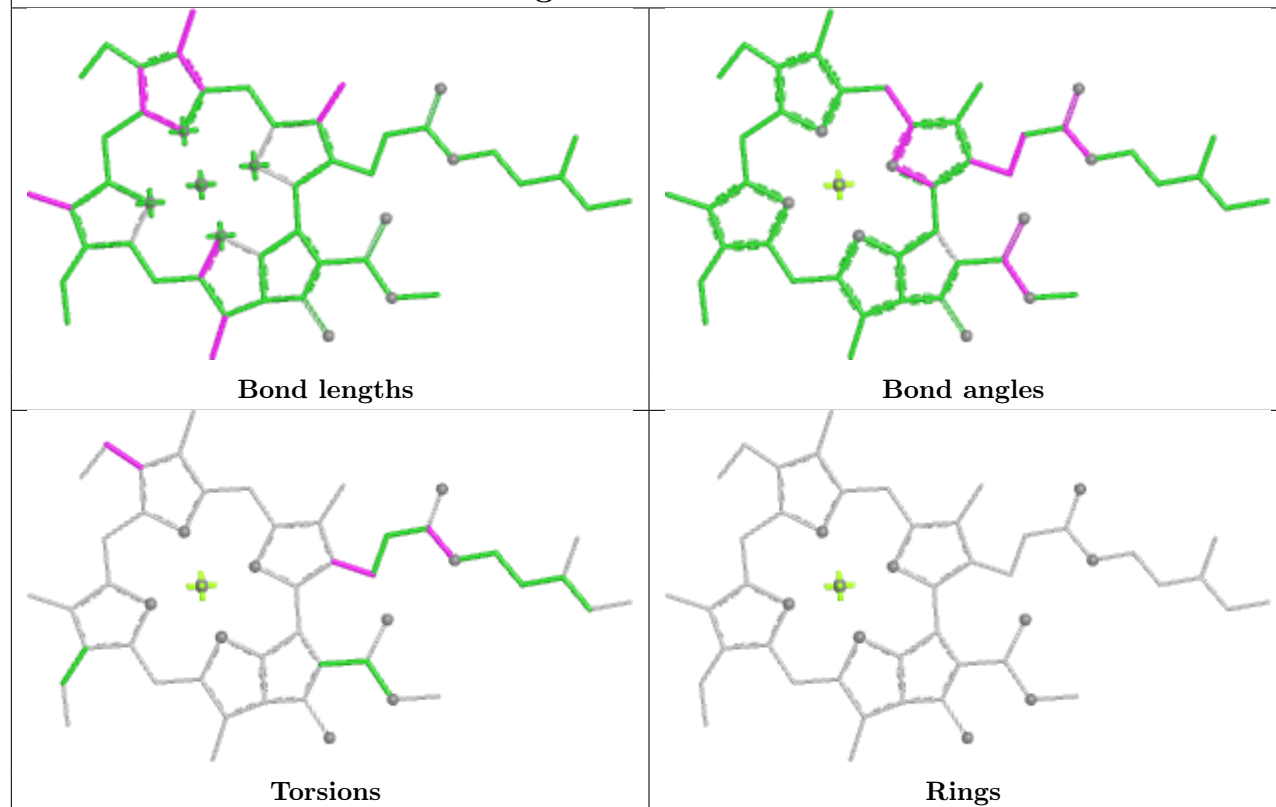
## Ligand CLA A 854



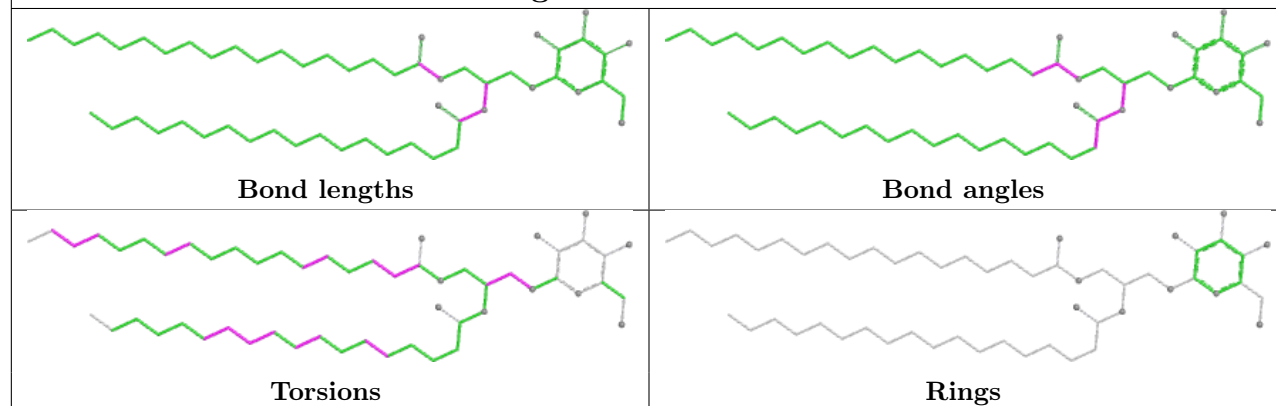




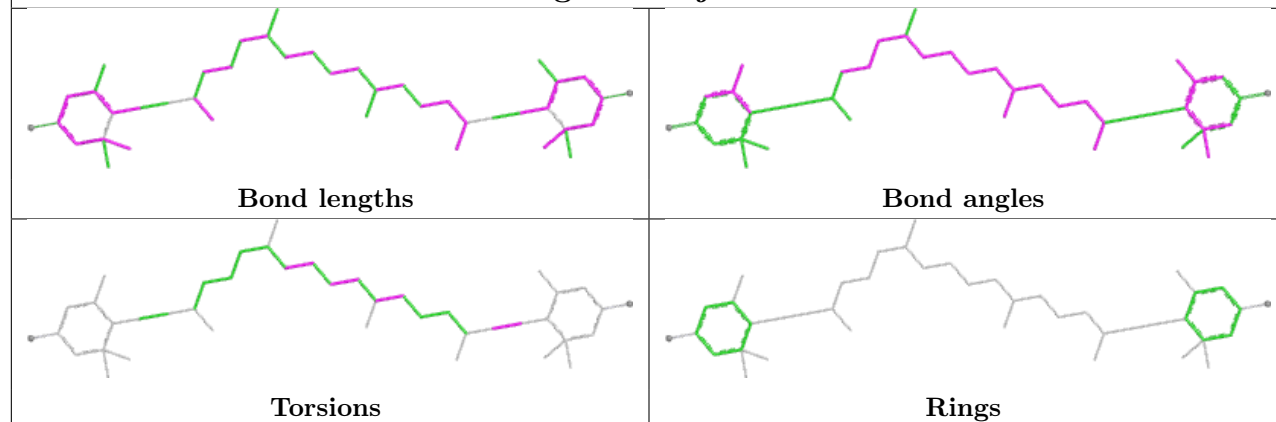
## Ligand CLA n 307

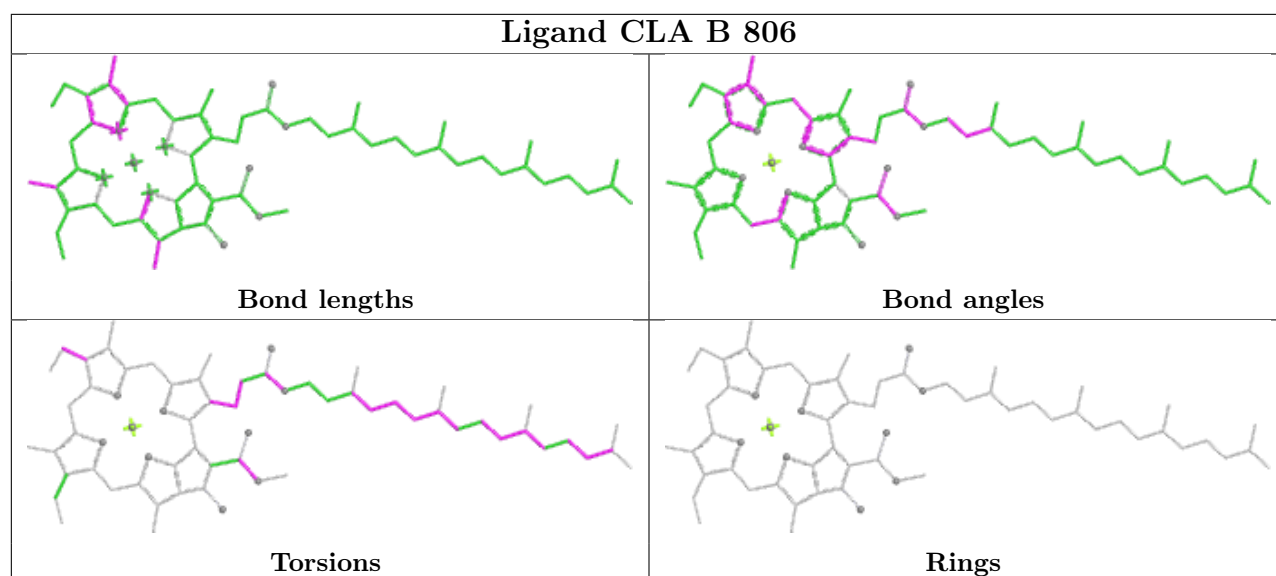
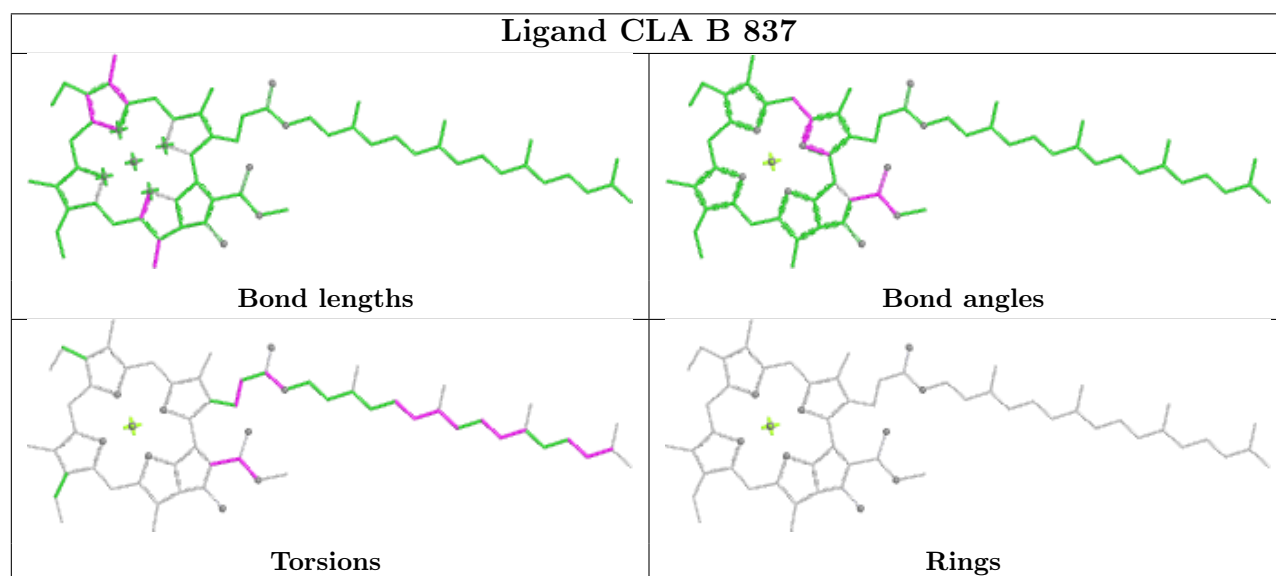
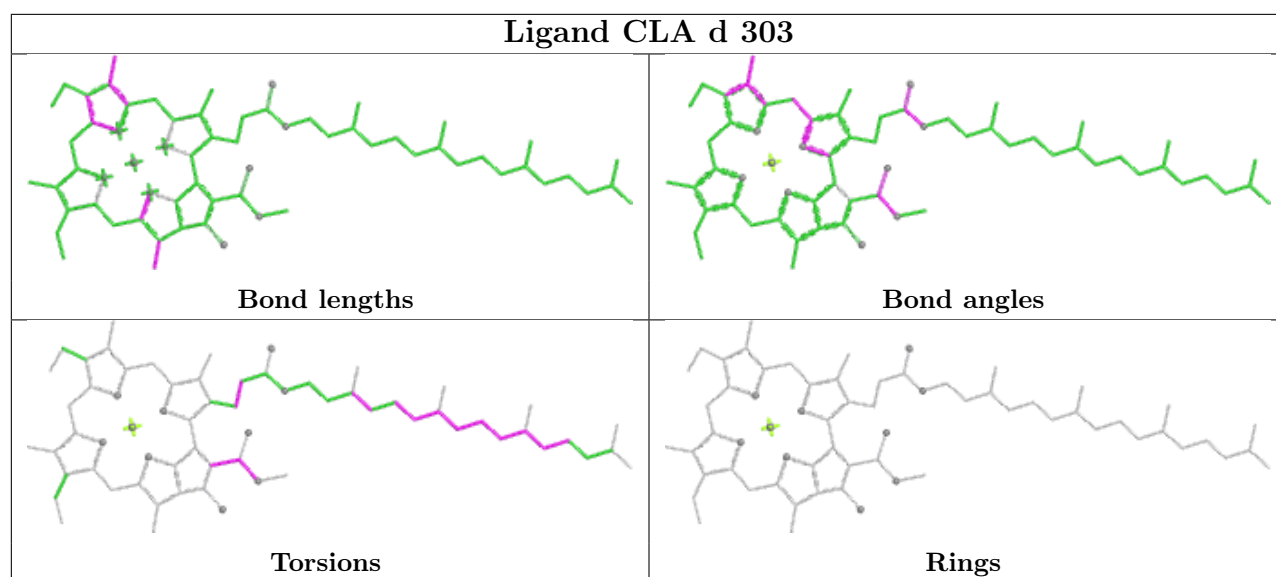


## Ligand LMG J 105

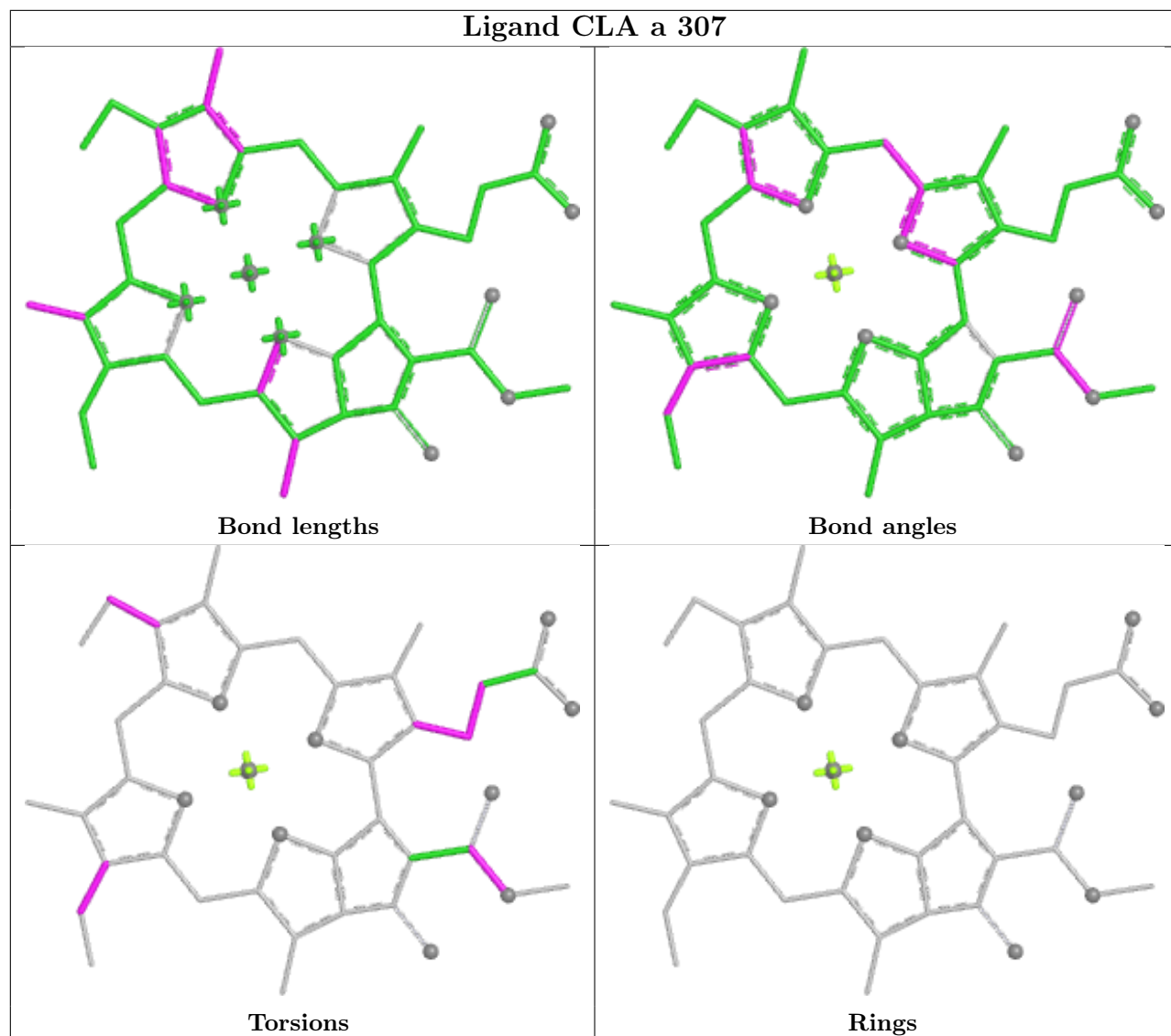


## Ligand II0 j 614

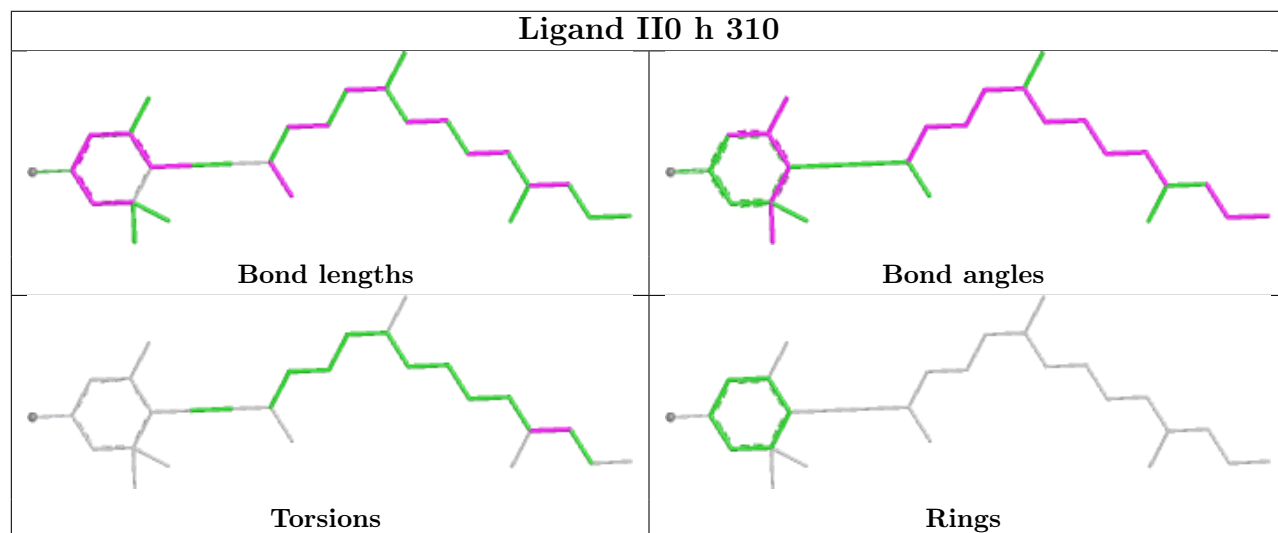




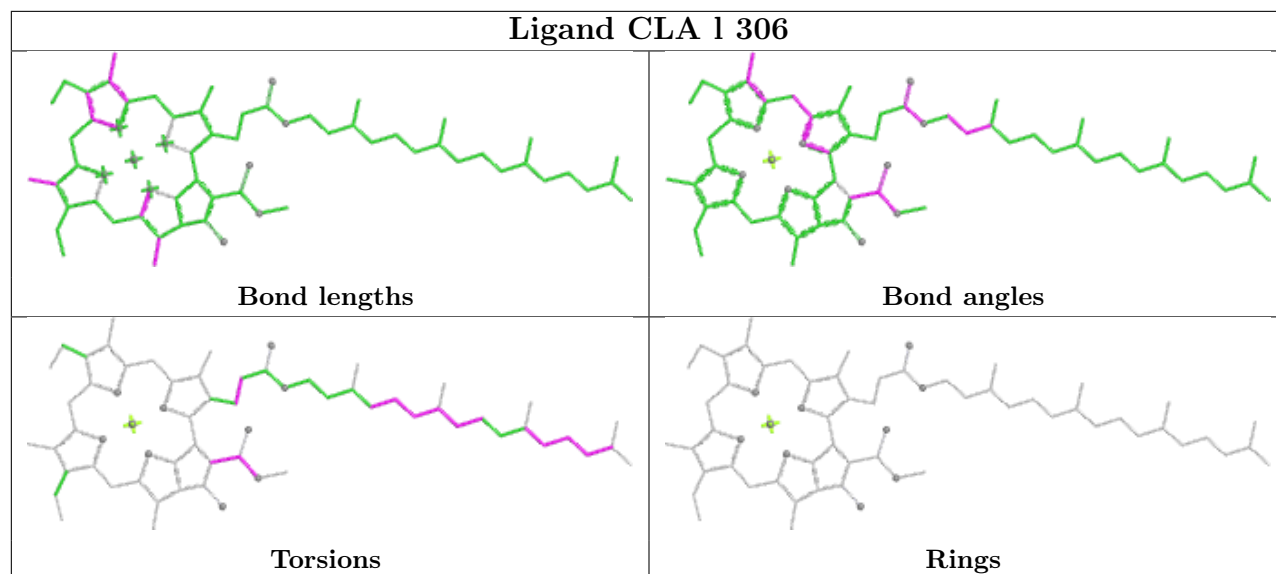
## Ligand CLA a 307



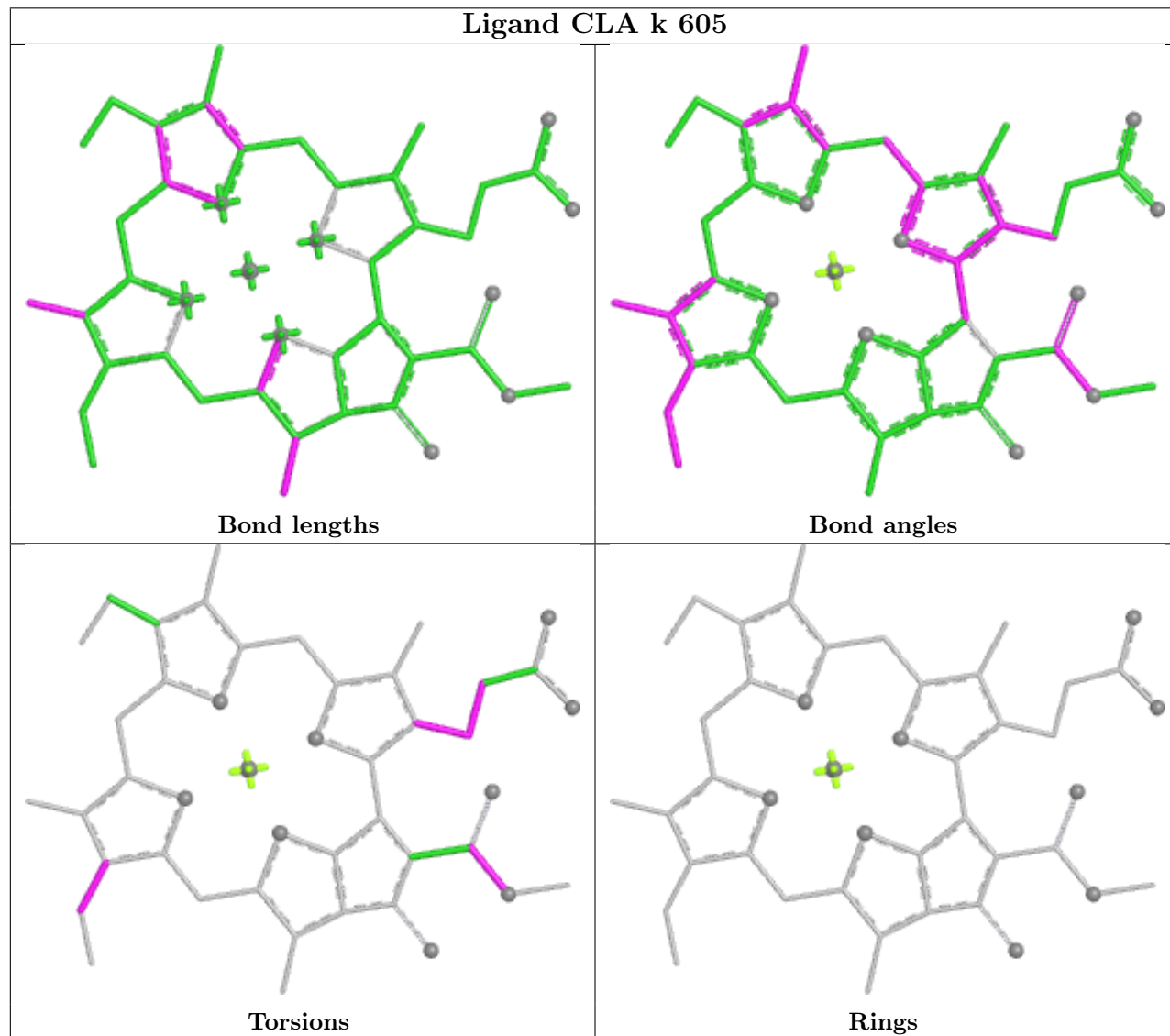
## Ligand II0 h 310



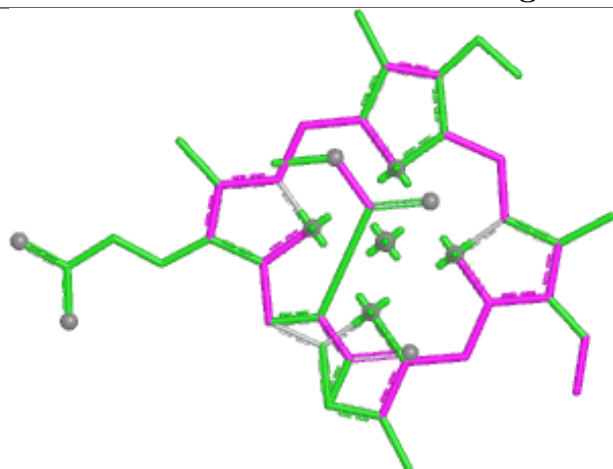
## Ligand CLA l 306



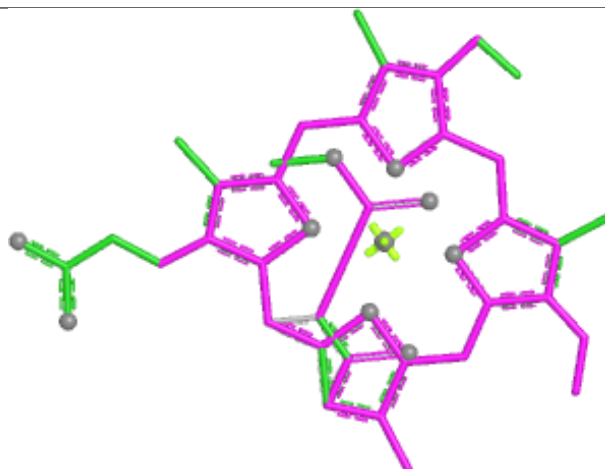
## Ligand CLA k 605



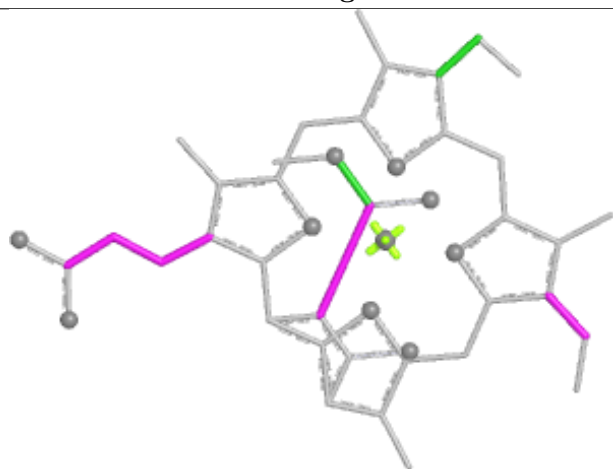
## Ligand KC2 d 310



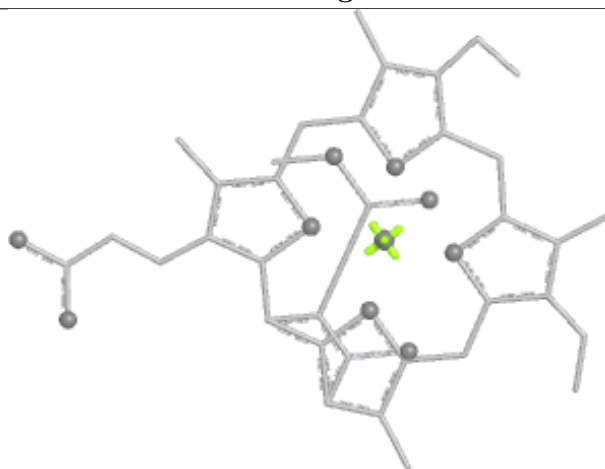
Bond lengths



Bond angles

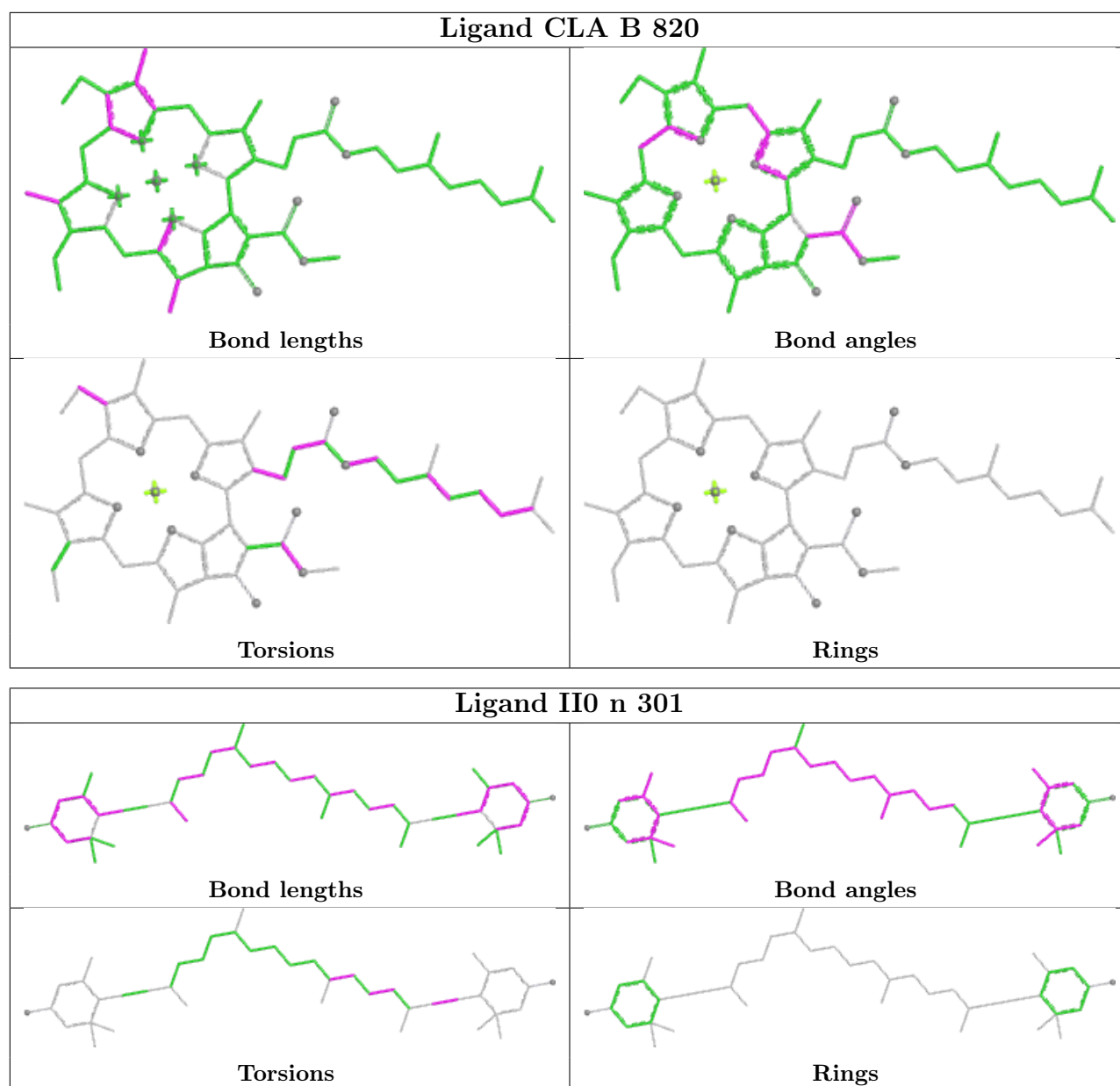


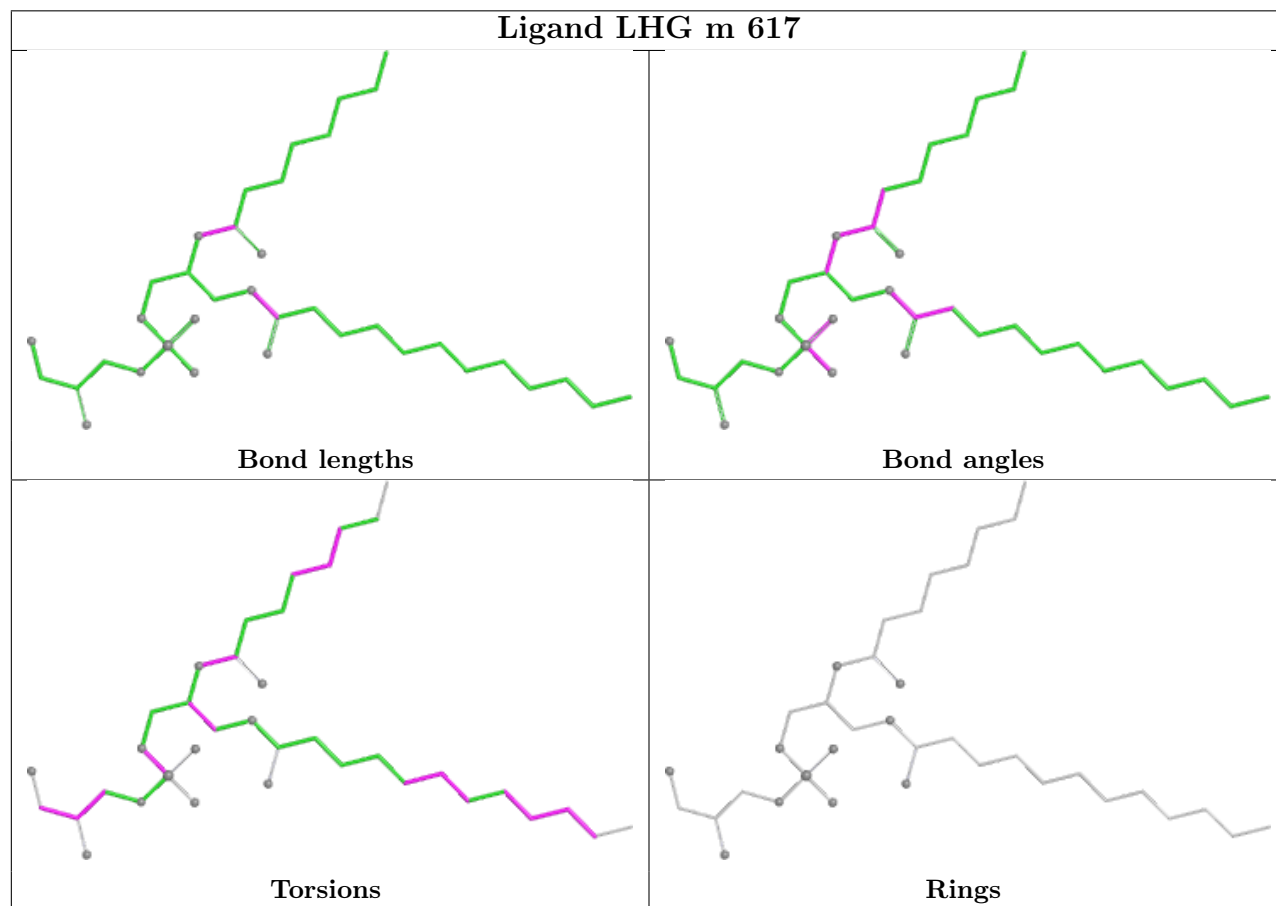
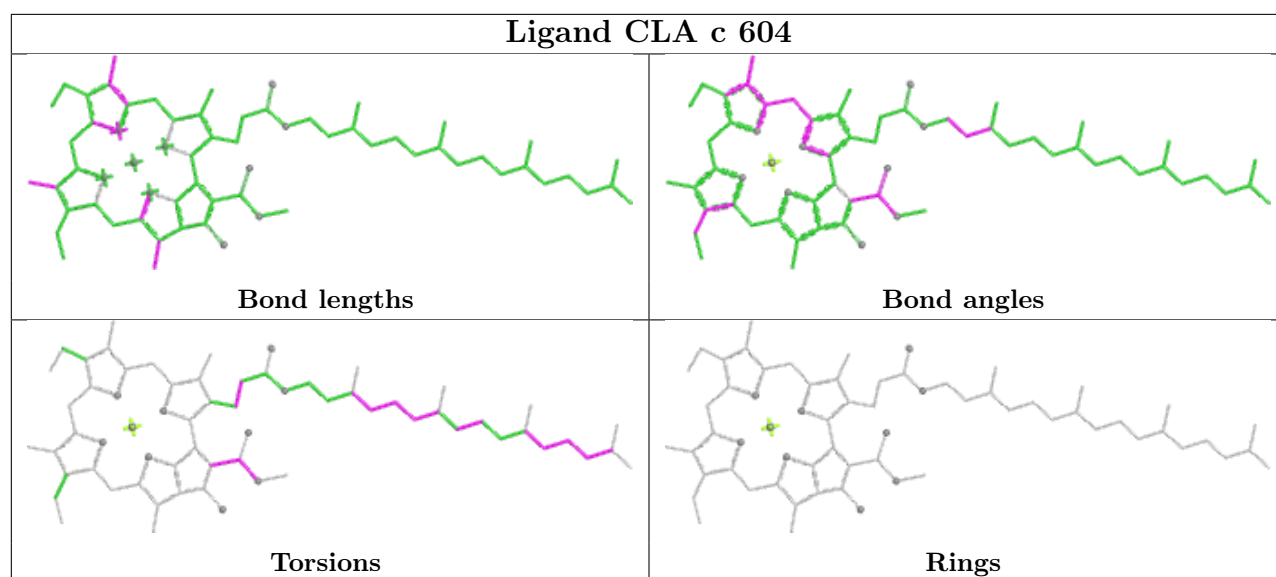
Torsions



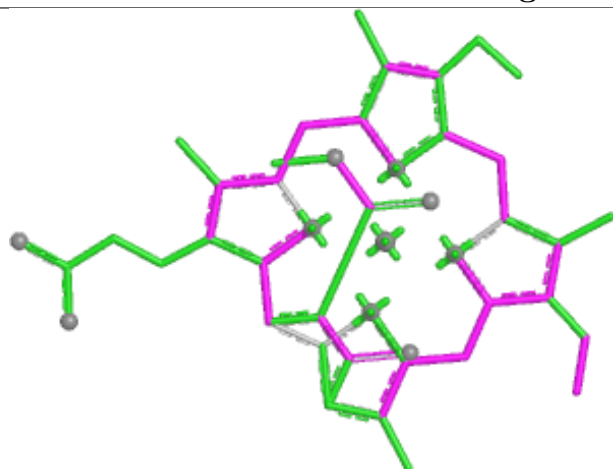
Rings



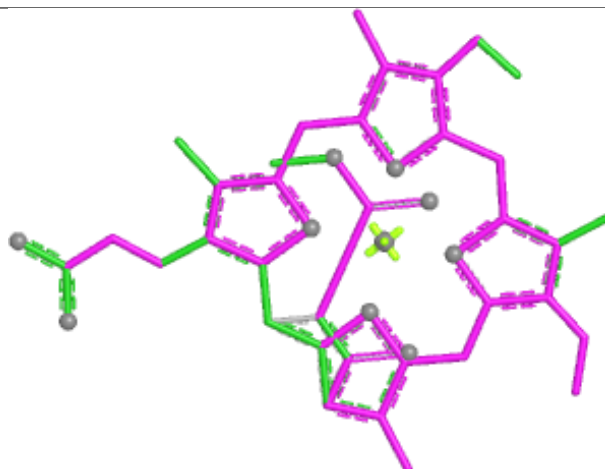




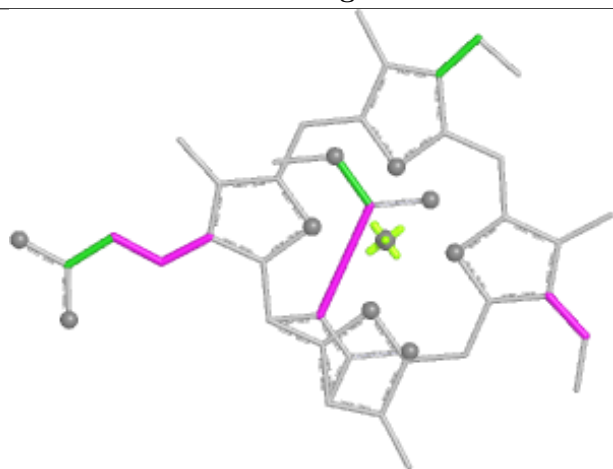
## Ligand KC2 n 313



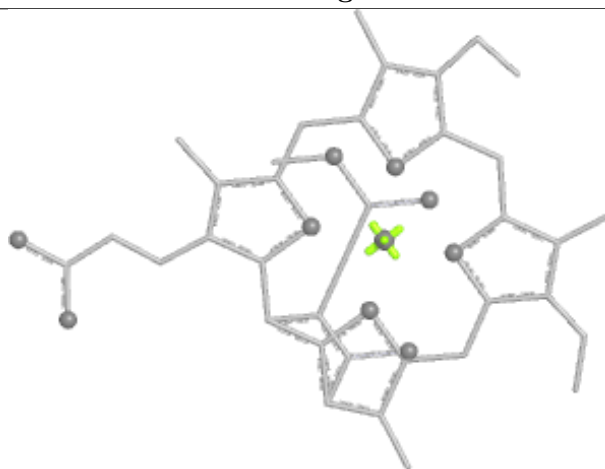
Bond lengths



Bond angles

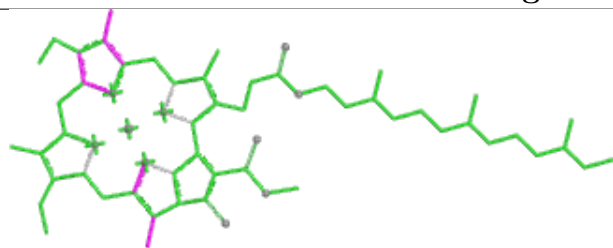


Torsions

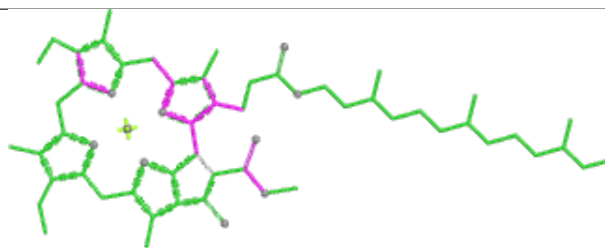


Rings

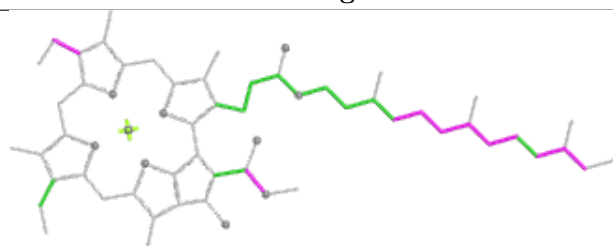
## Ligand CLA l 310



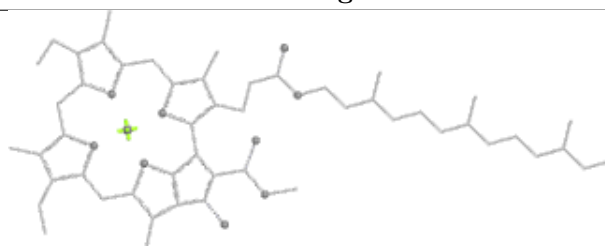
Bond lengths



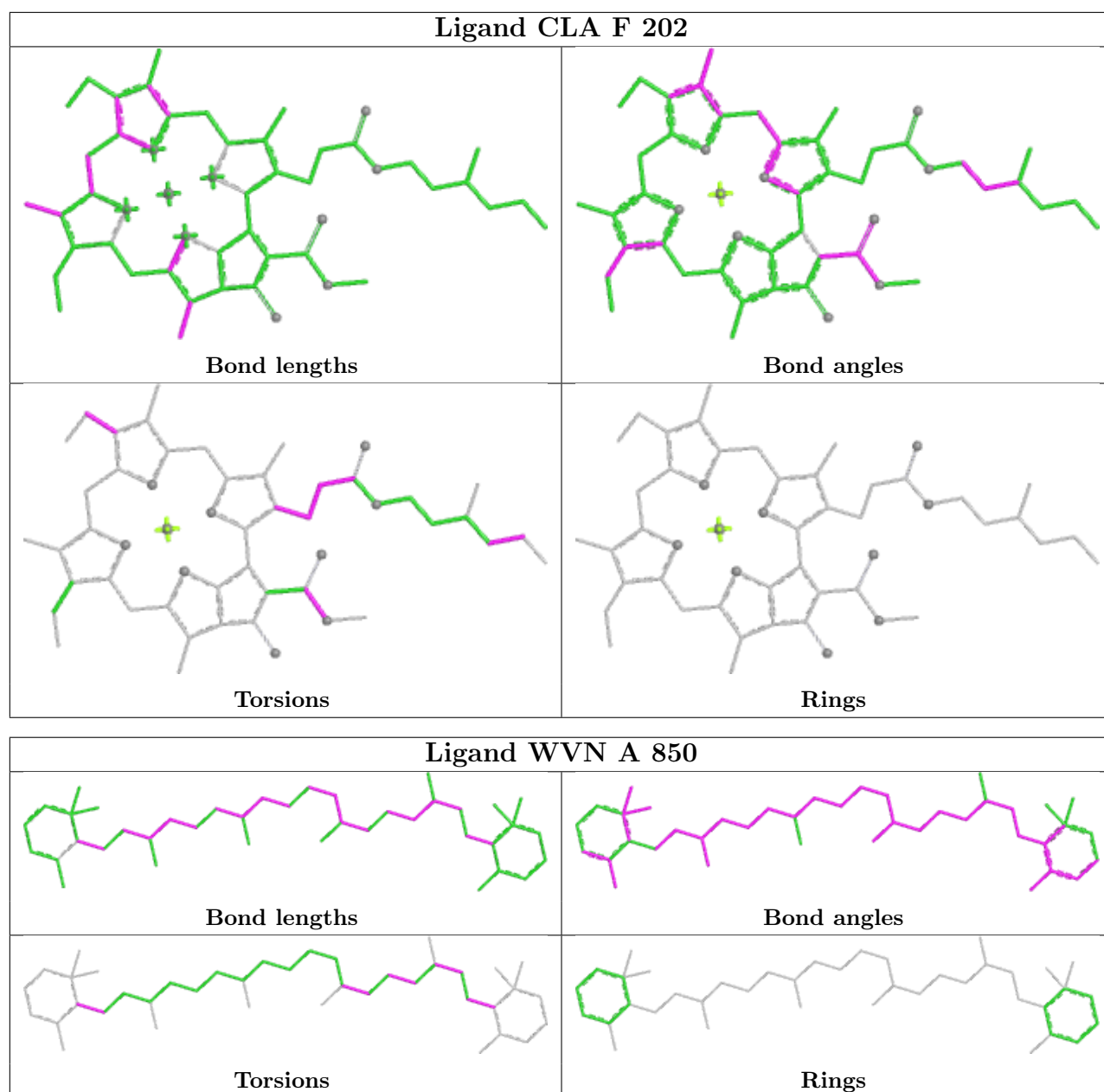
Bond angles



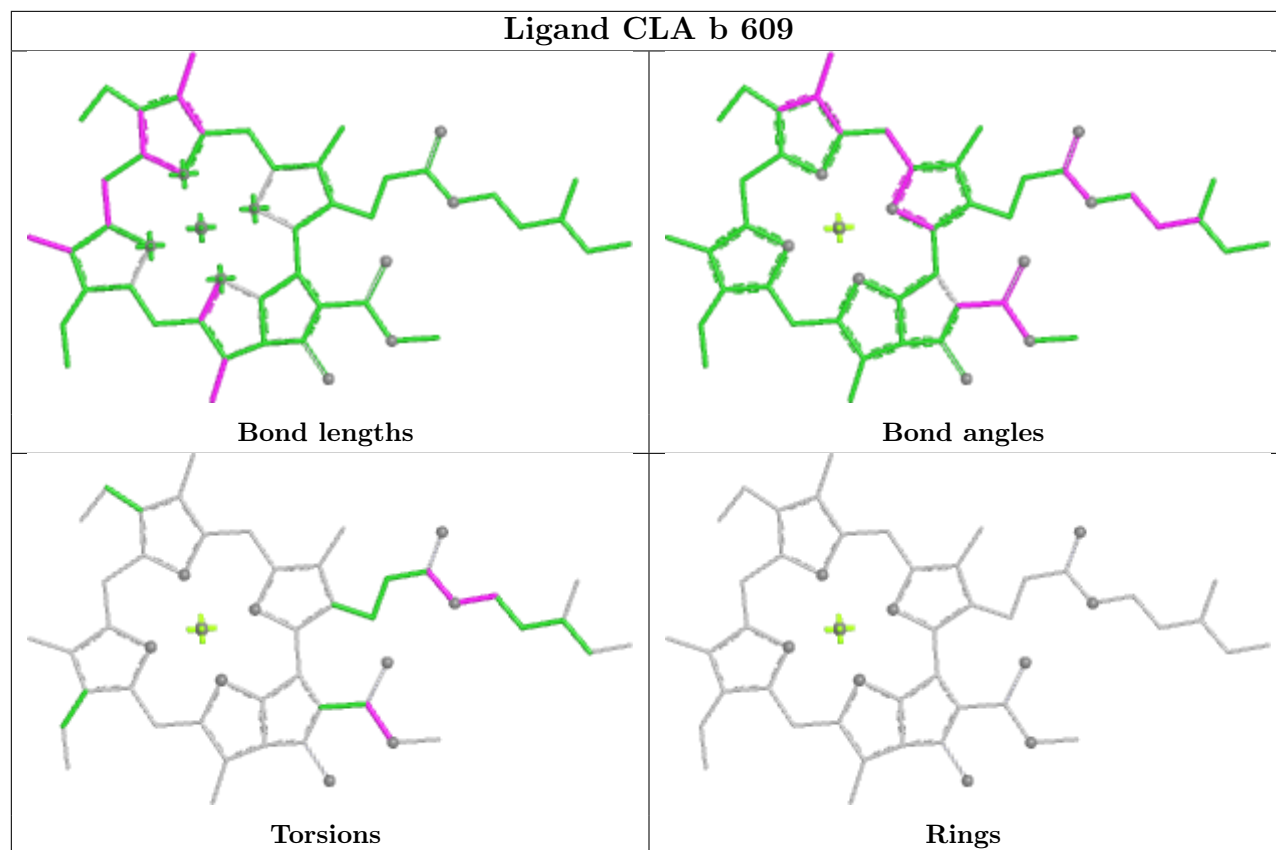
Torsions



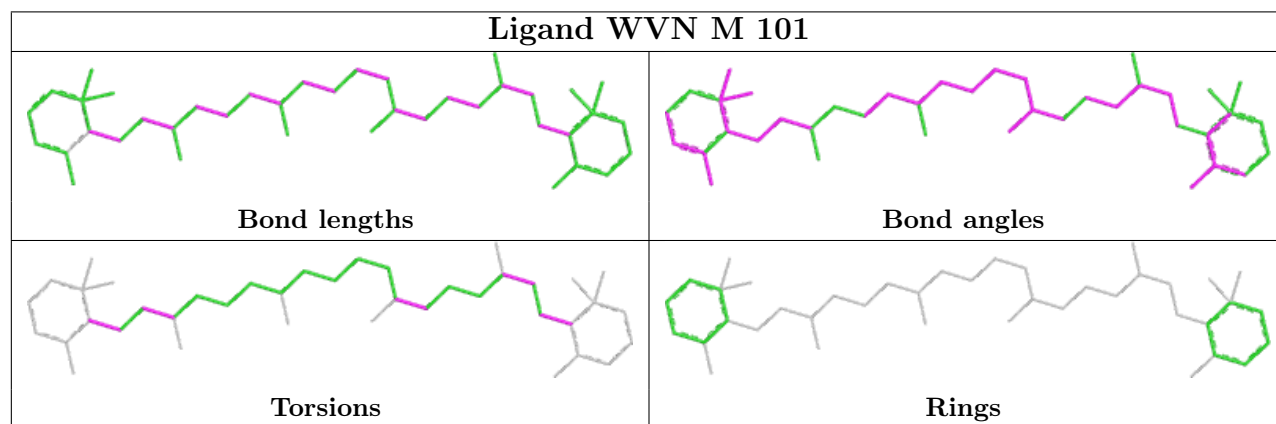
Rings

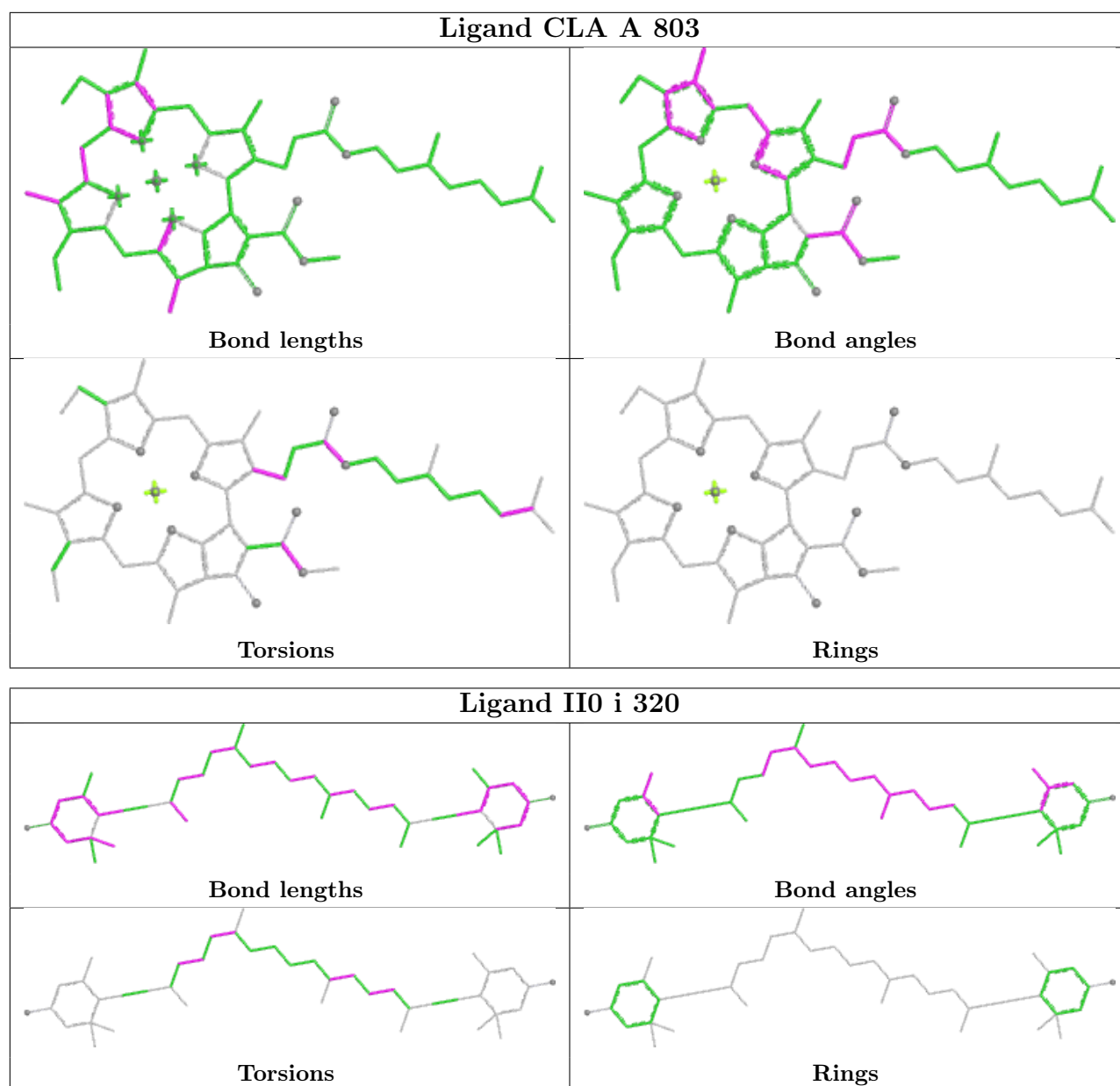


## Ligand CLA b 609

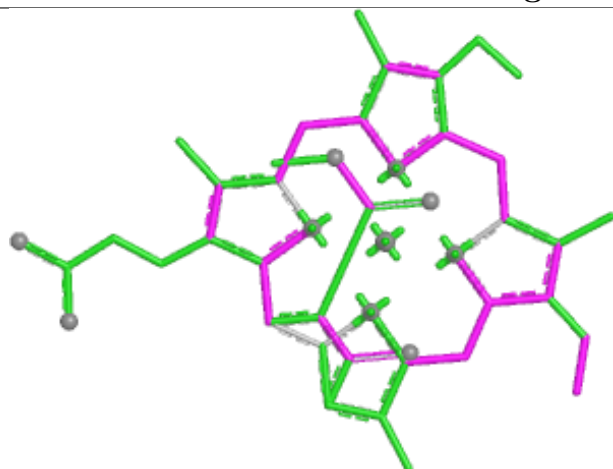


## Ligand WVN M 101

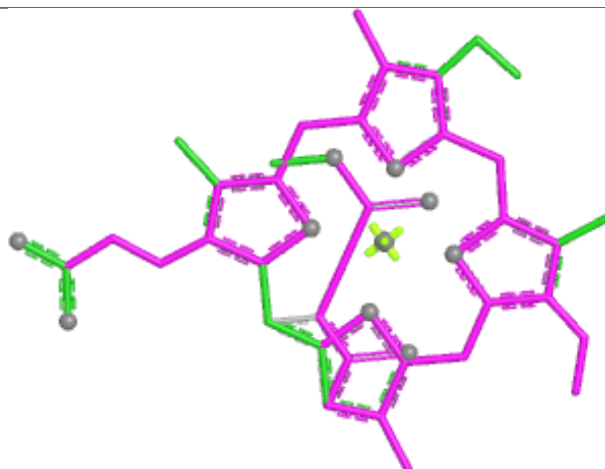




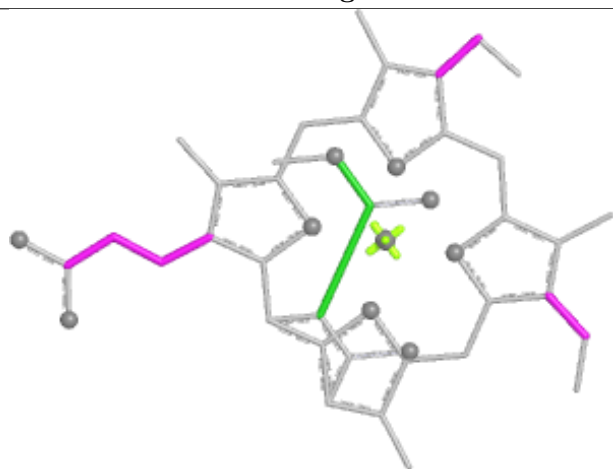
## Ligand KC2 i 310



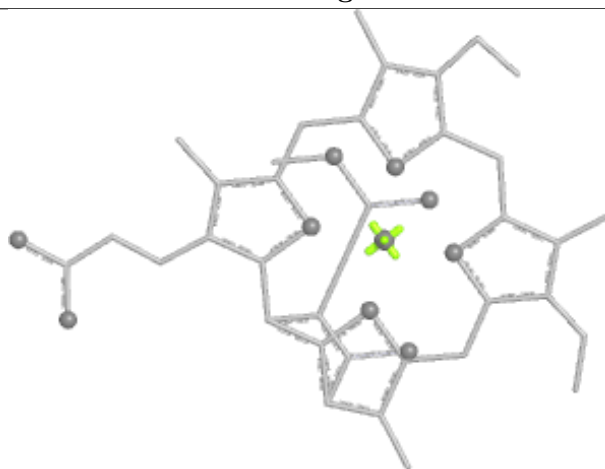
Bond lengths



Bond angles

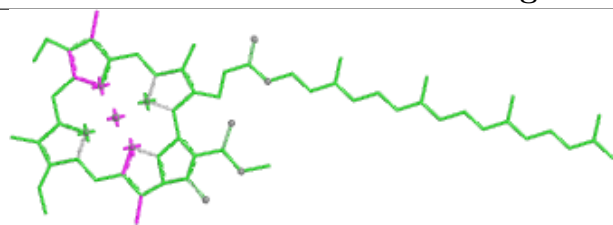


Torsions

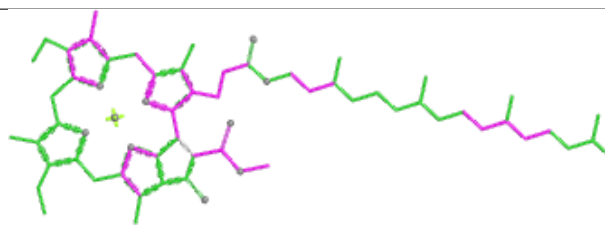


Rings

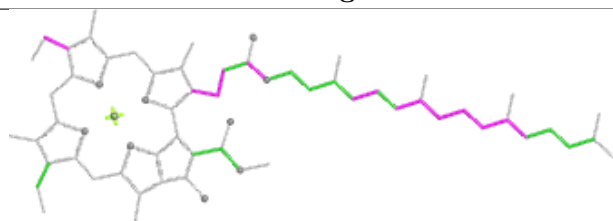
## Ligand CLA s 202



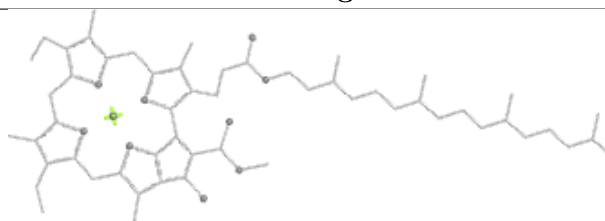
Bond lengths



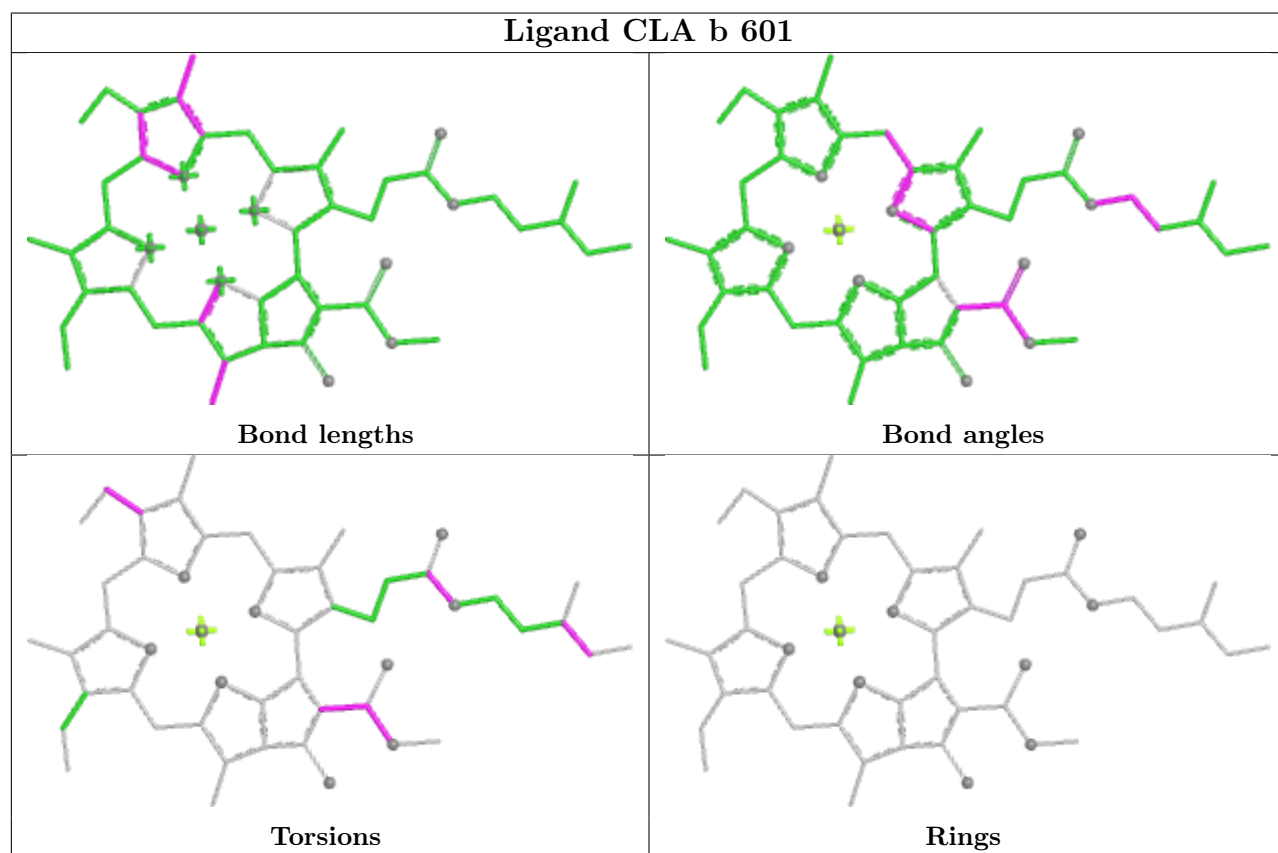
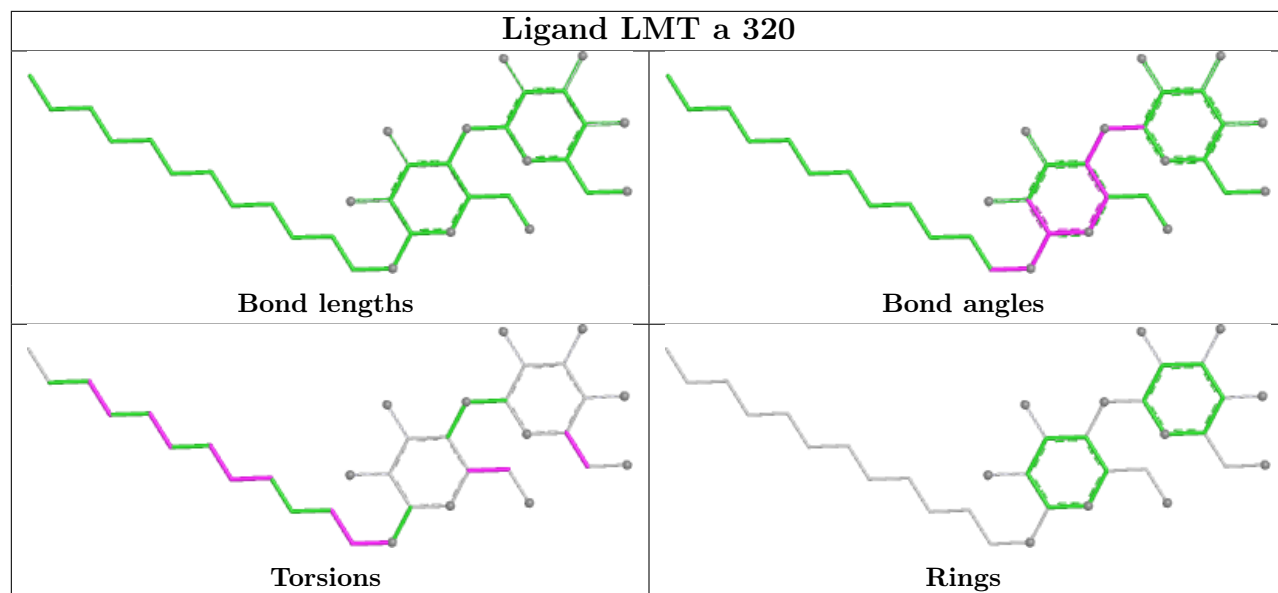
Bond angles



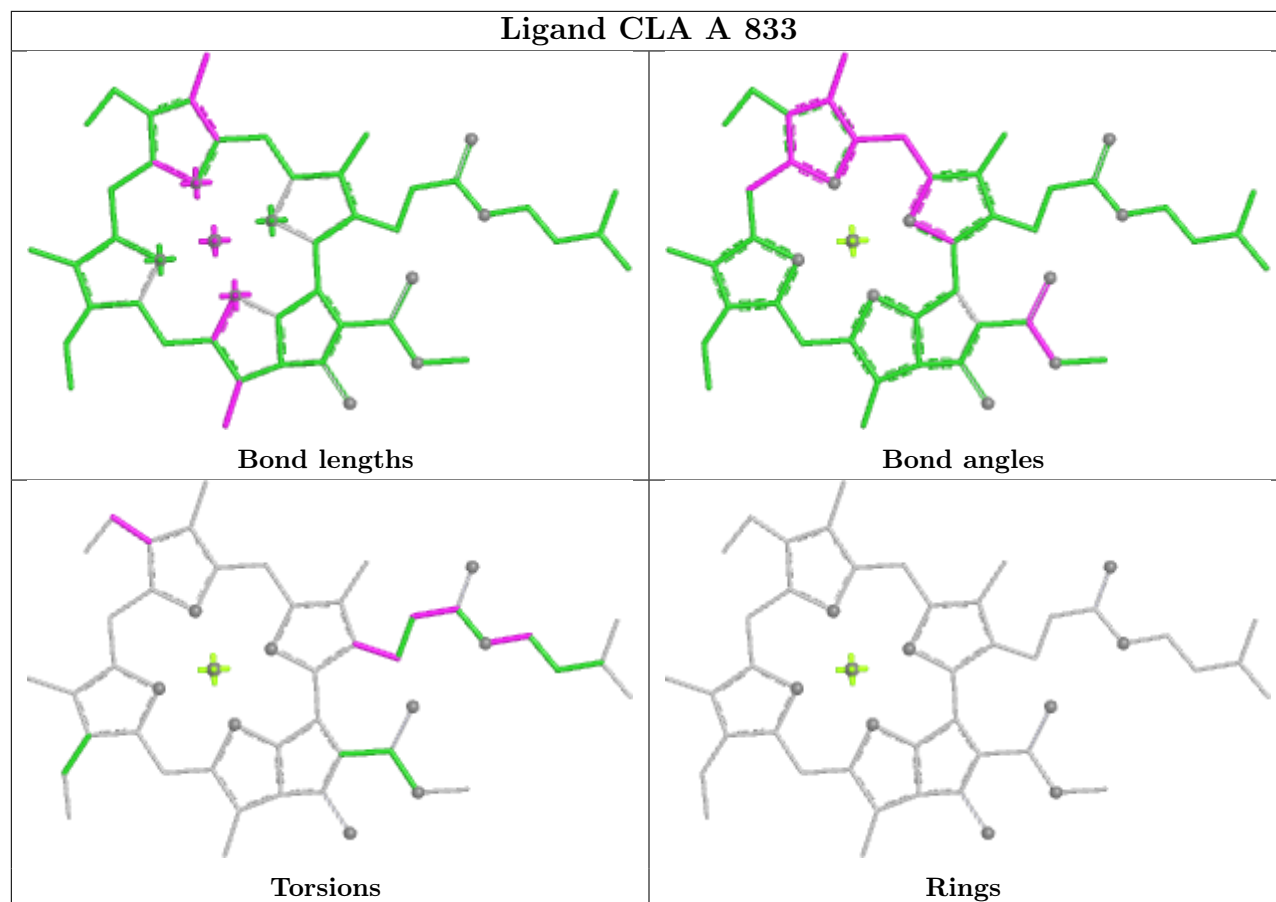
Torsions

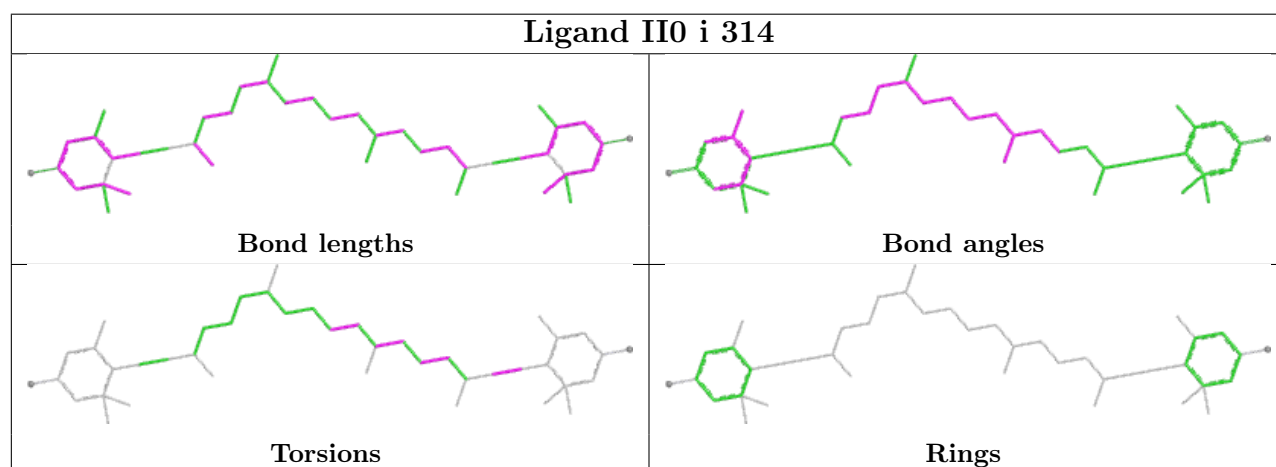
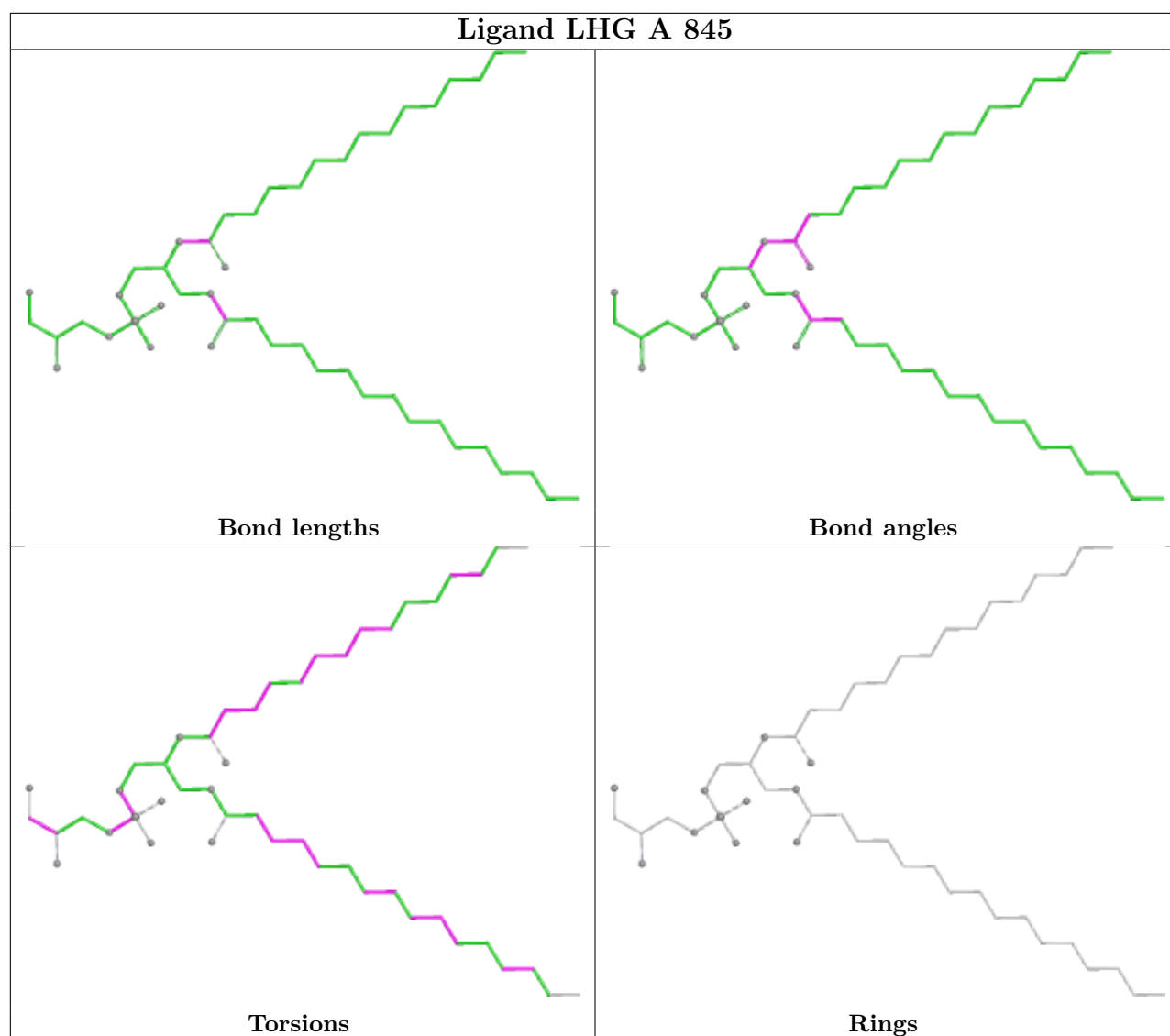


Rings

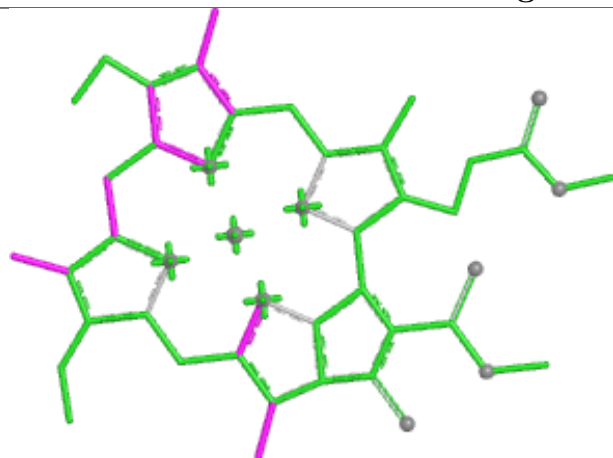




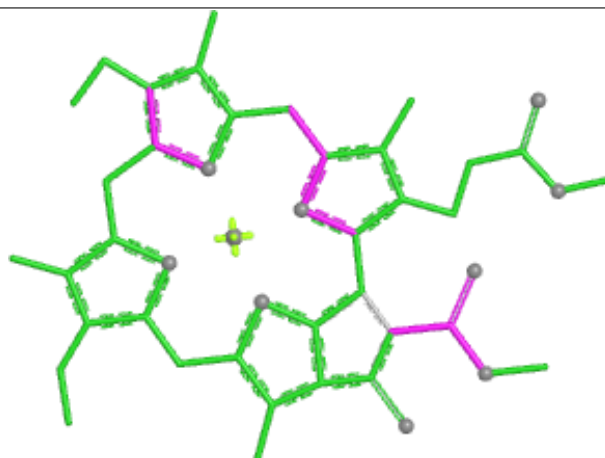




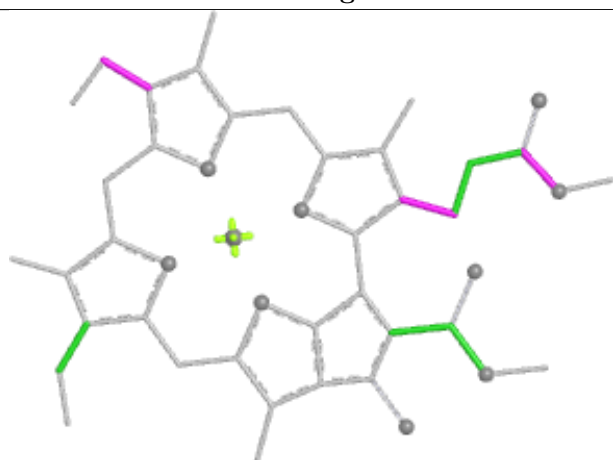
## Ligand CLA d 307



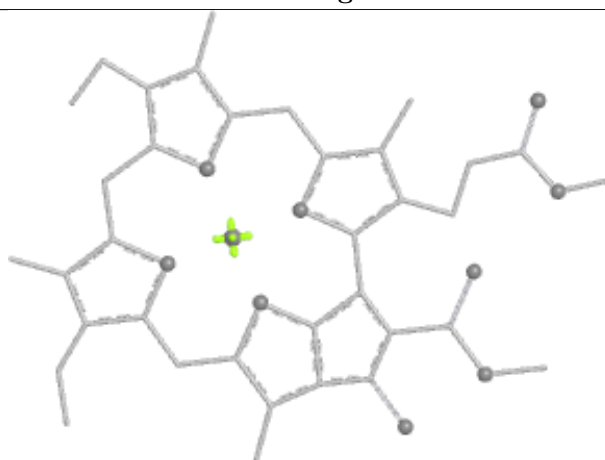
Bond lengths



Bond angles

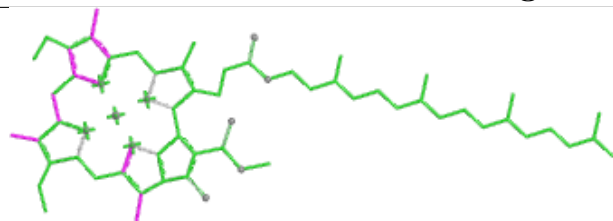


Torsions

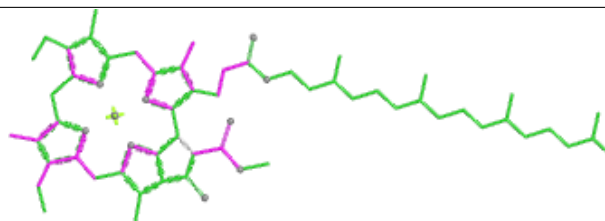


Rings

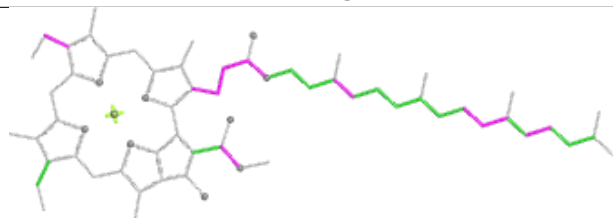
## Ligand CLA c 608



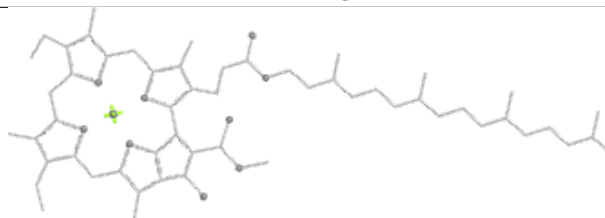
Bond lengths



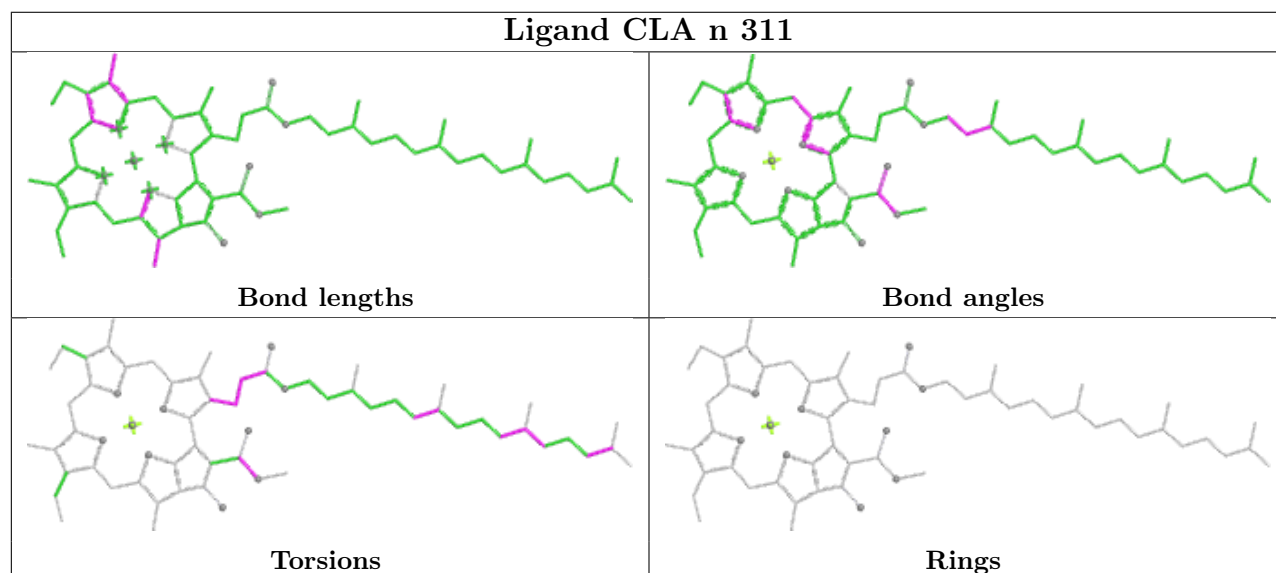
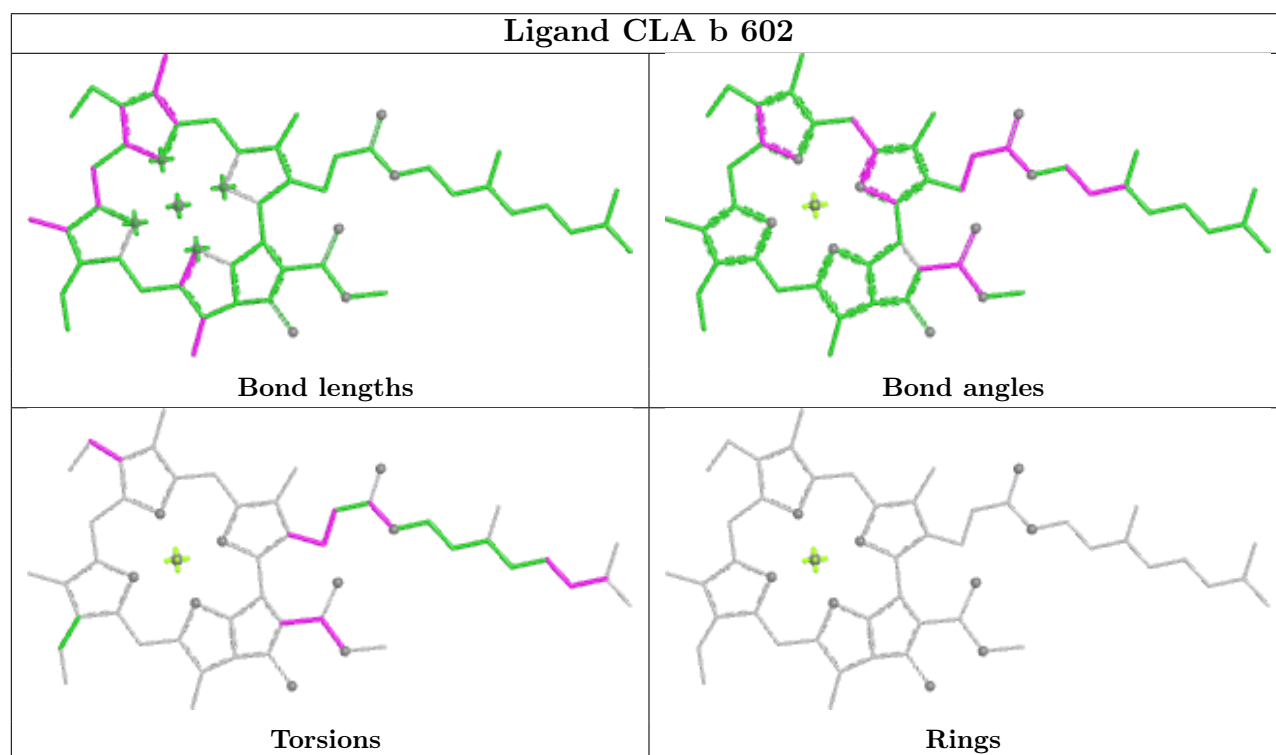
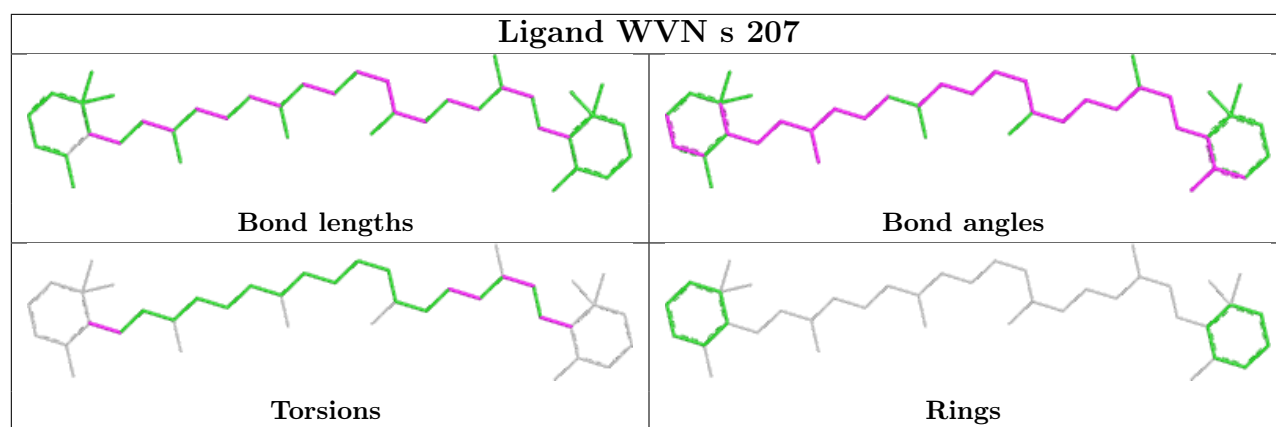
Bond angles

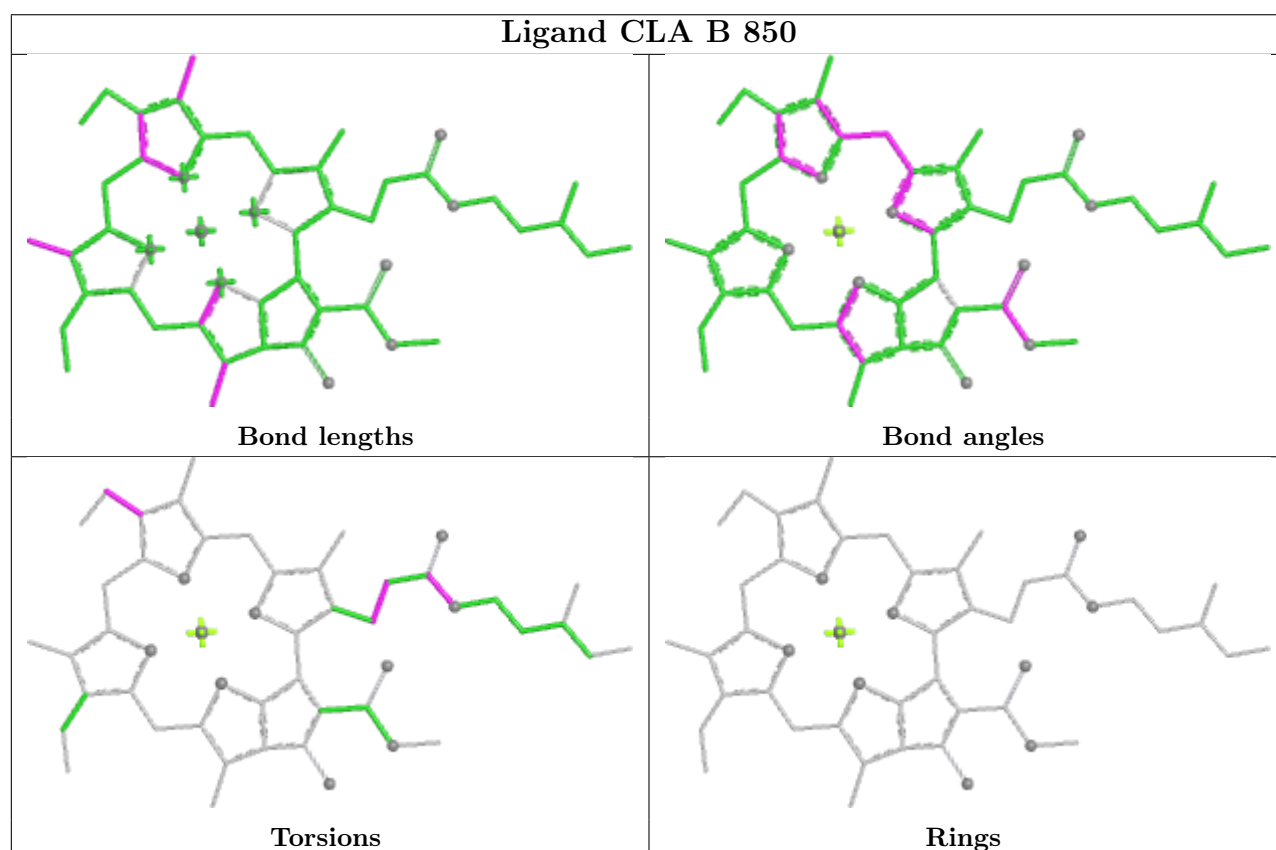
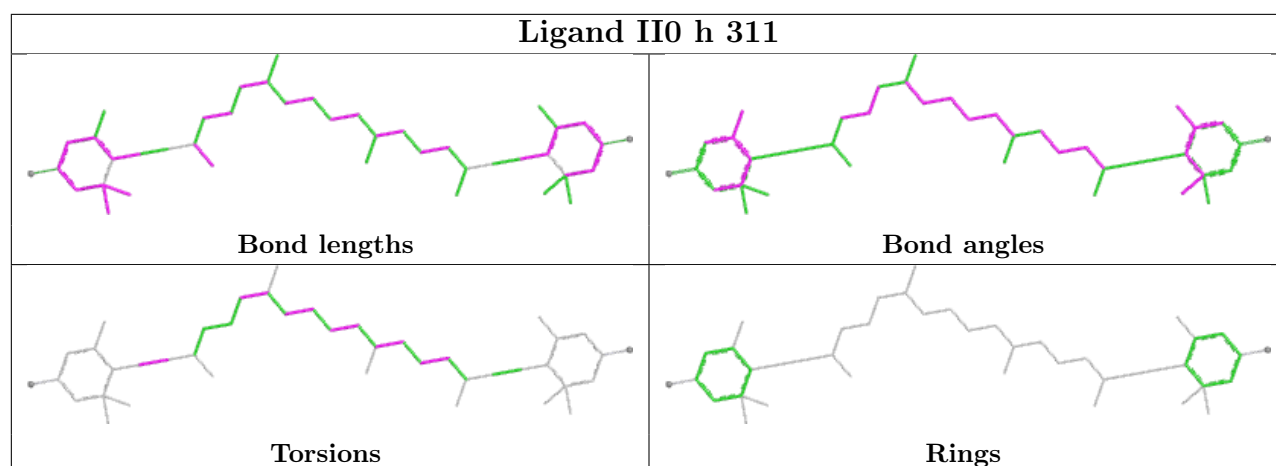


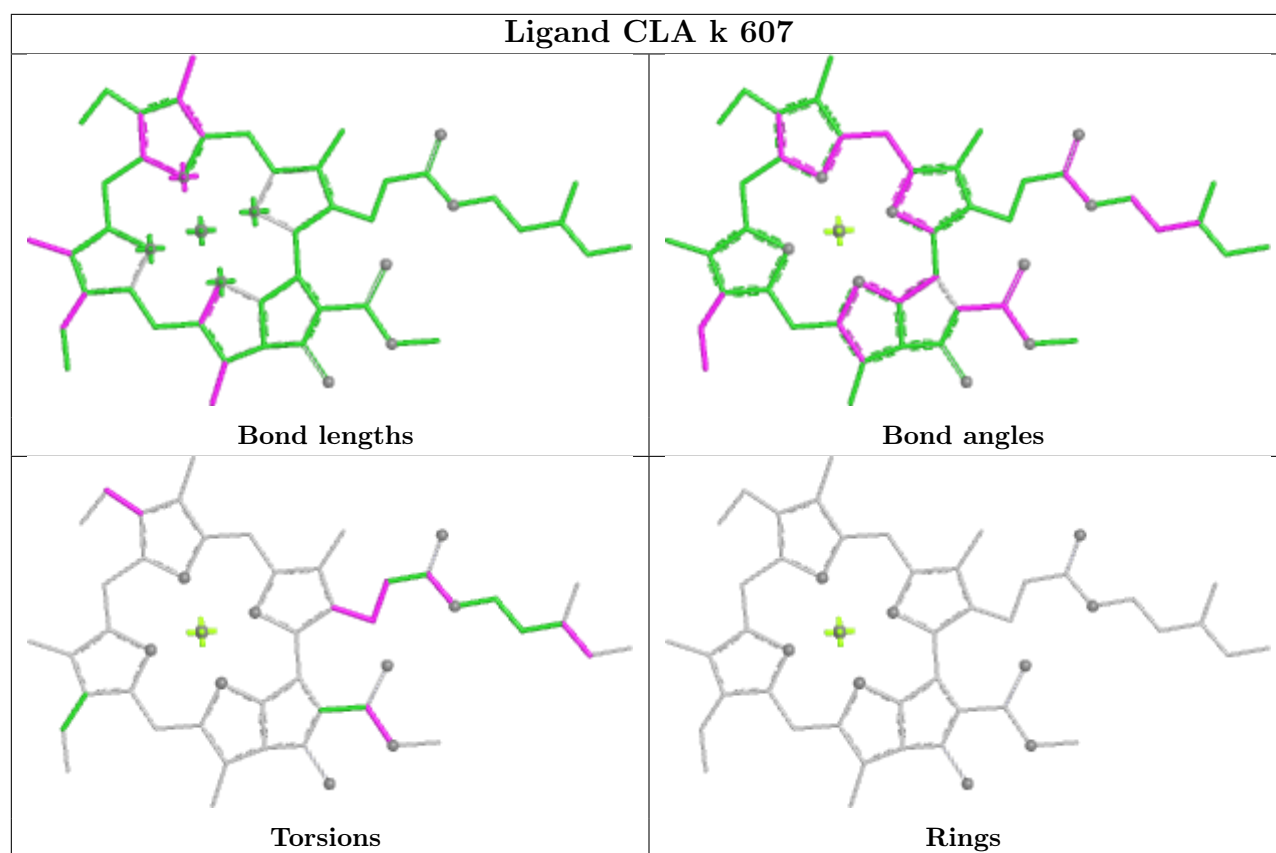
Torsions

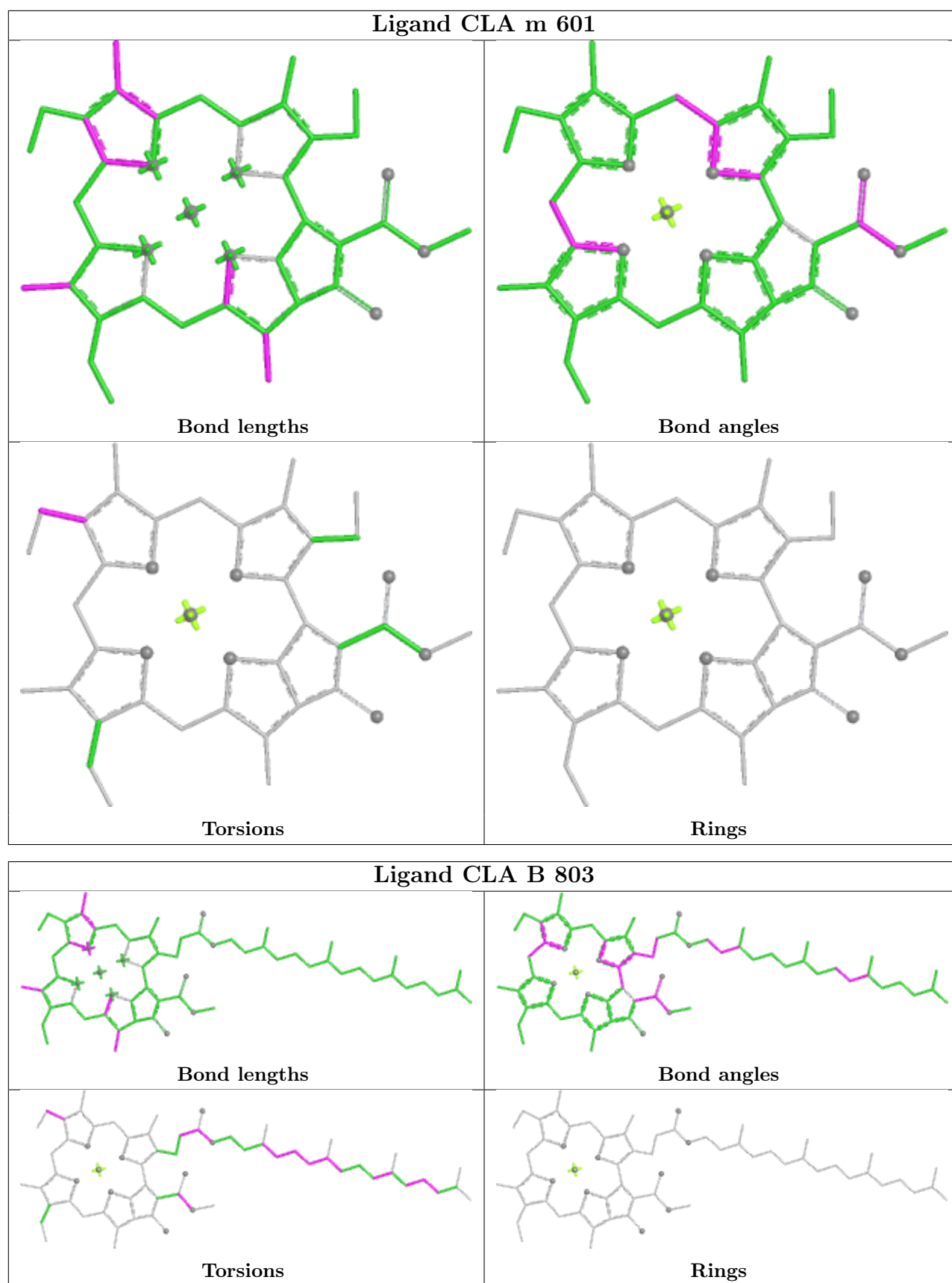


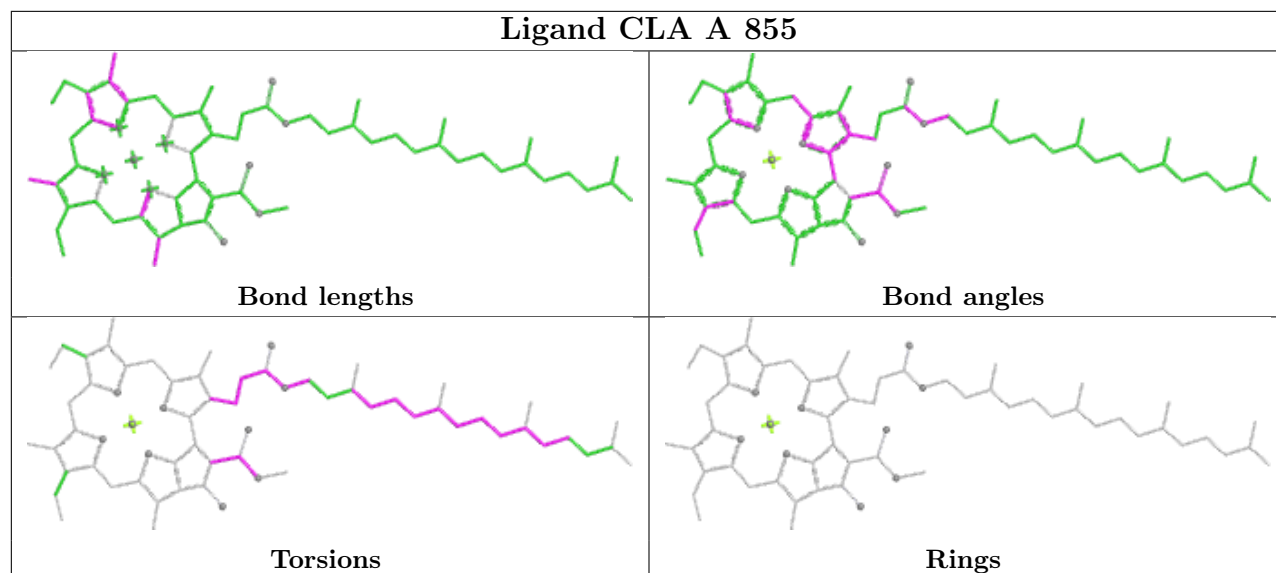
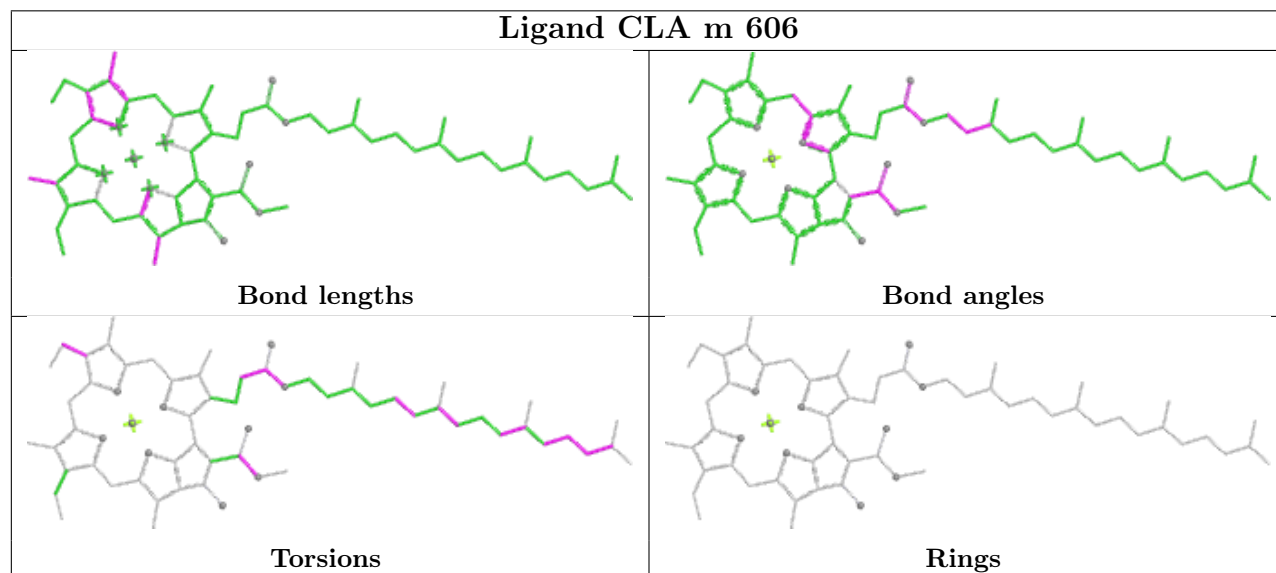
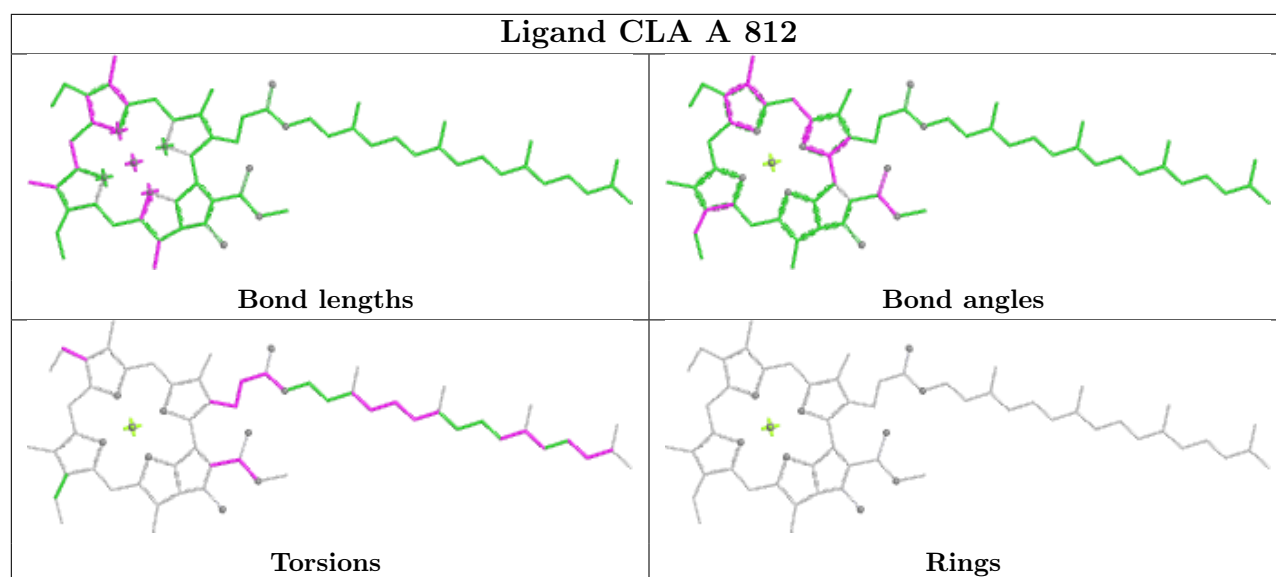
Rings





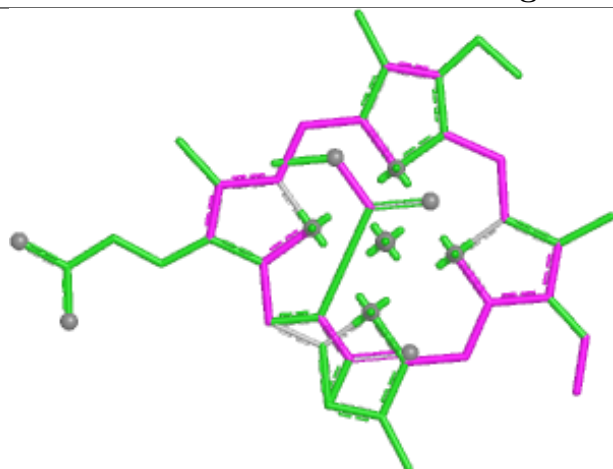




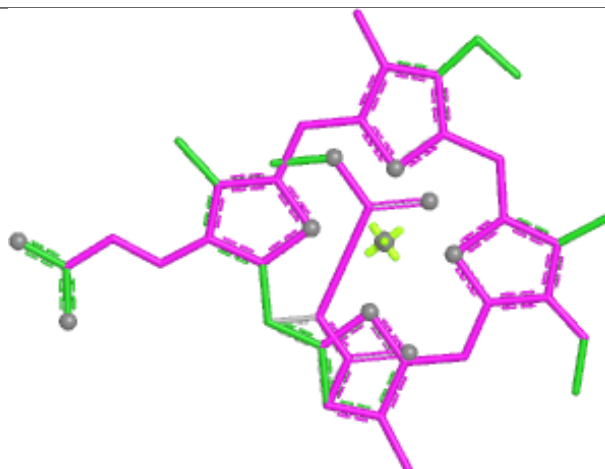




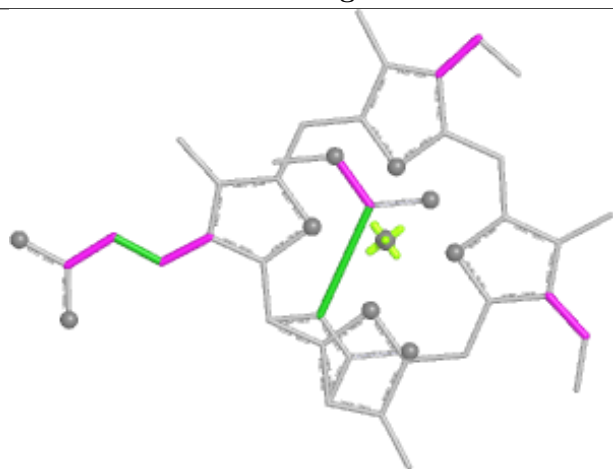
## Ligand KC2 k 612



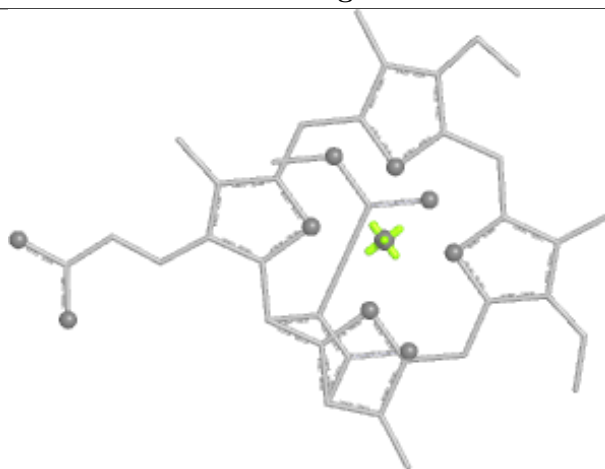
Bond lengths



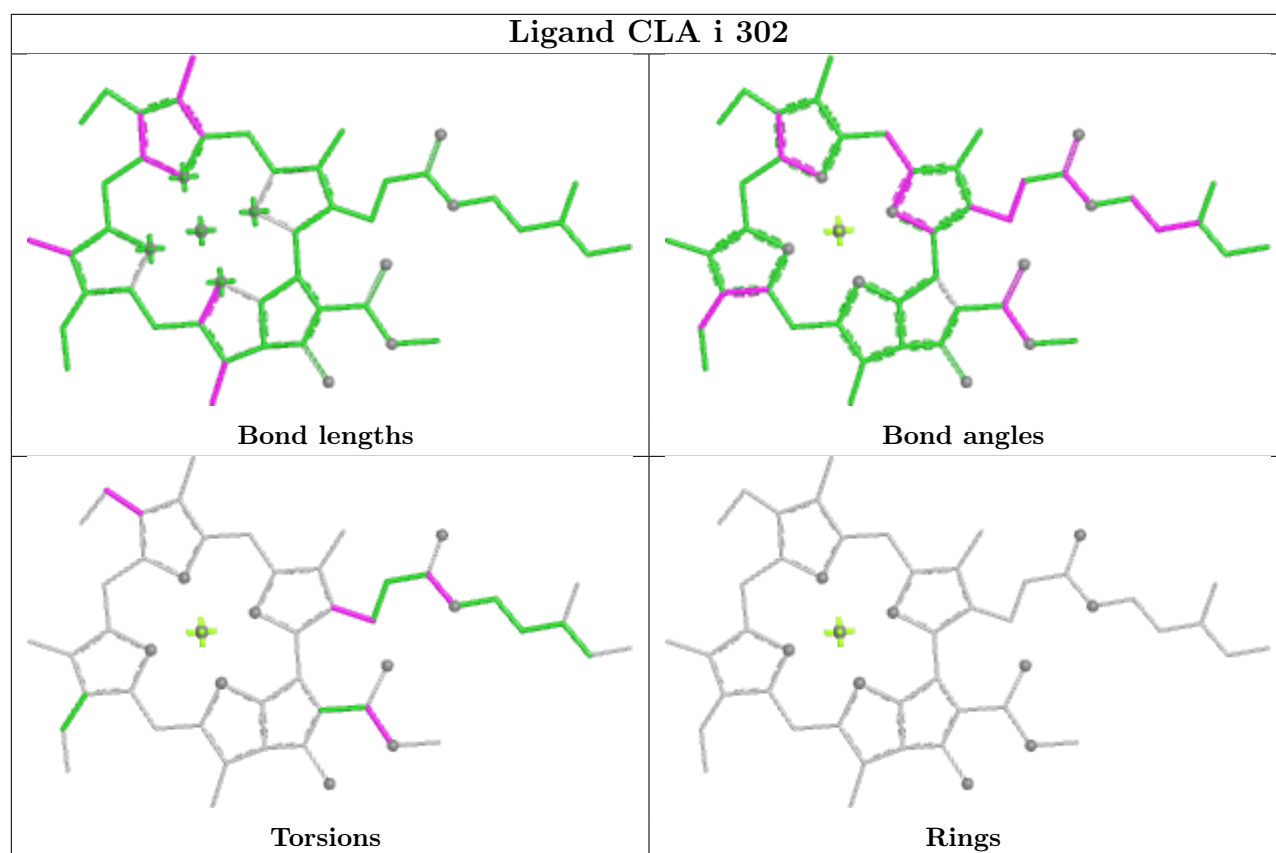
Bond angles



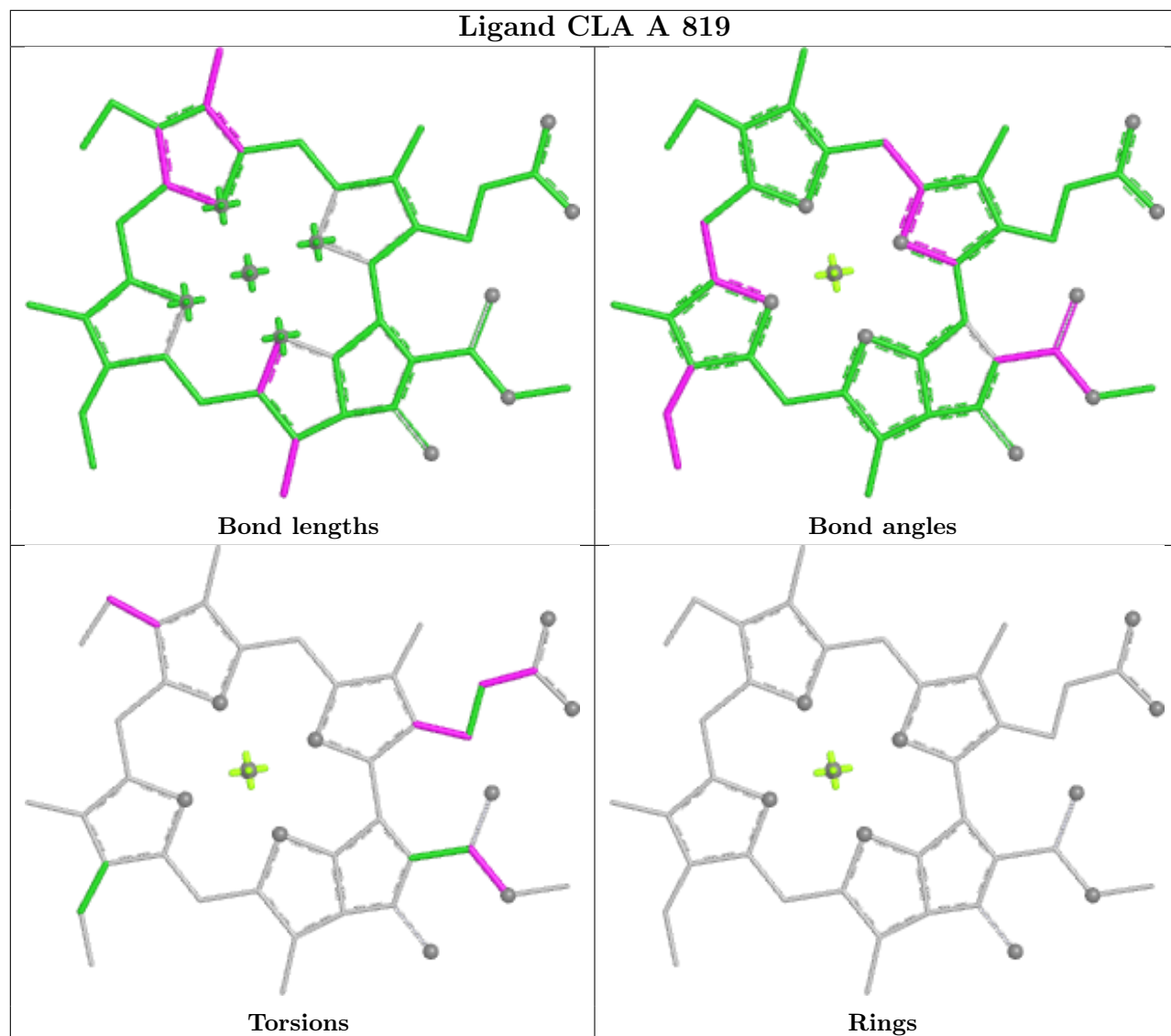
Torsions

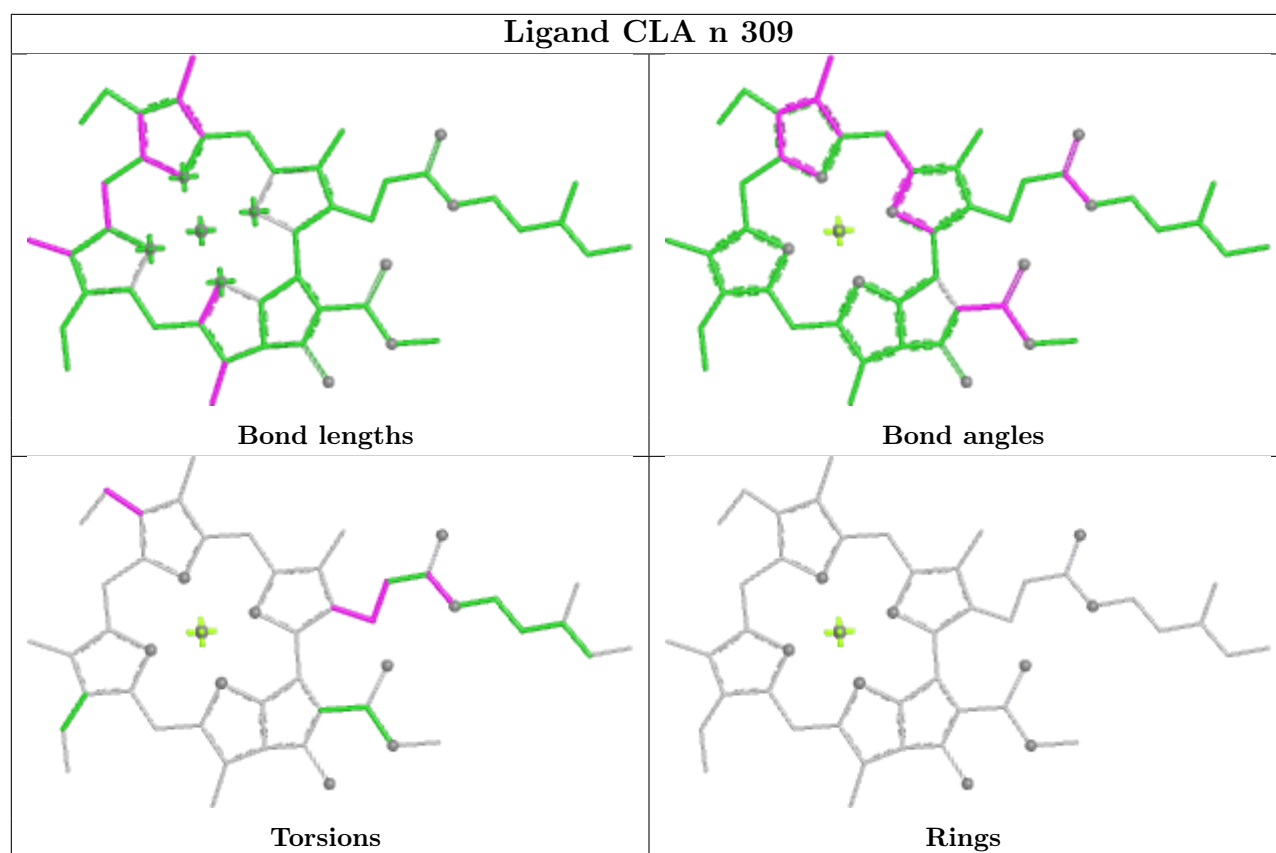


Rings

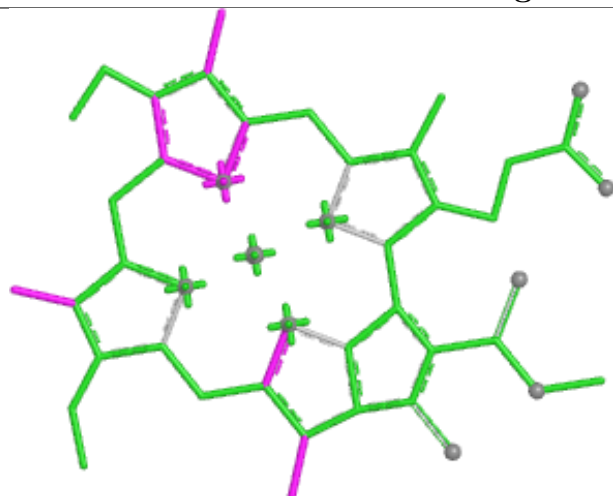


## Ligand CLA A 819

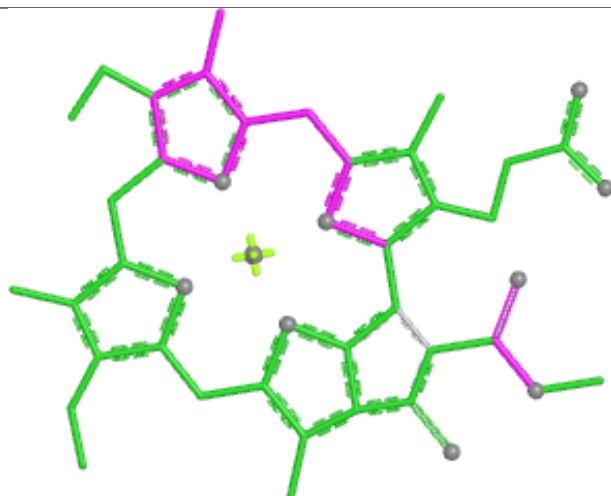




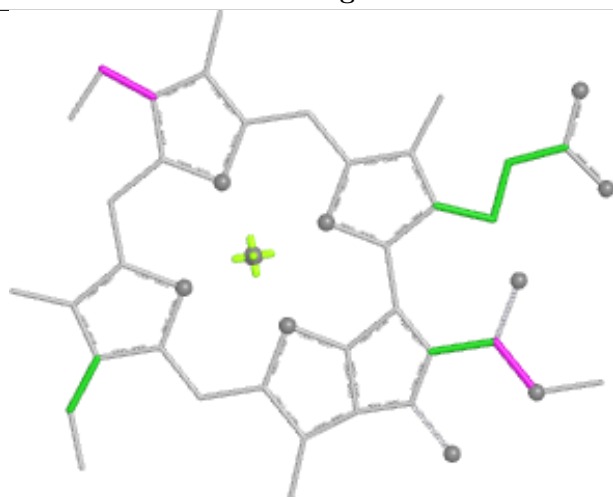
## Ligand CLA B 831



Bond lengths



Bond angles

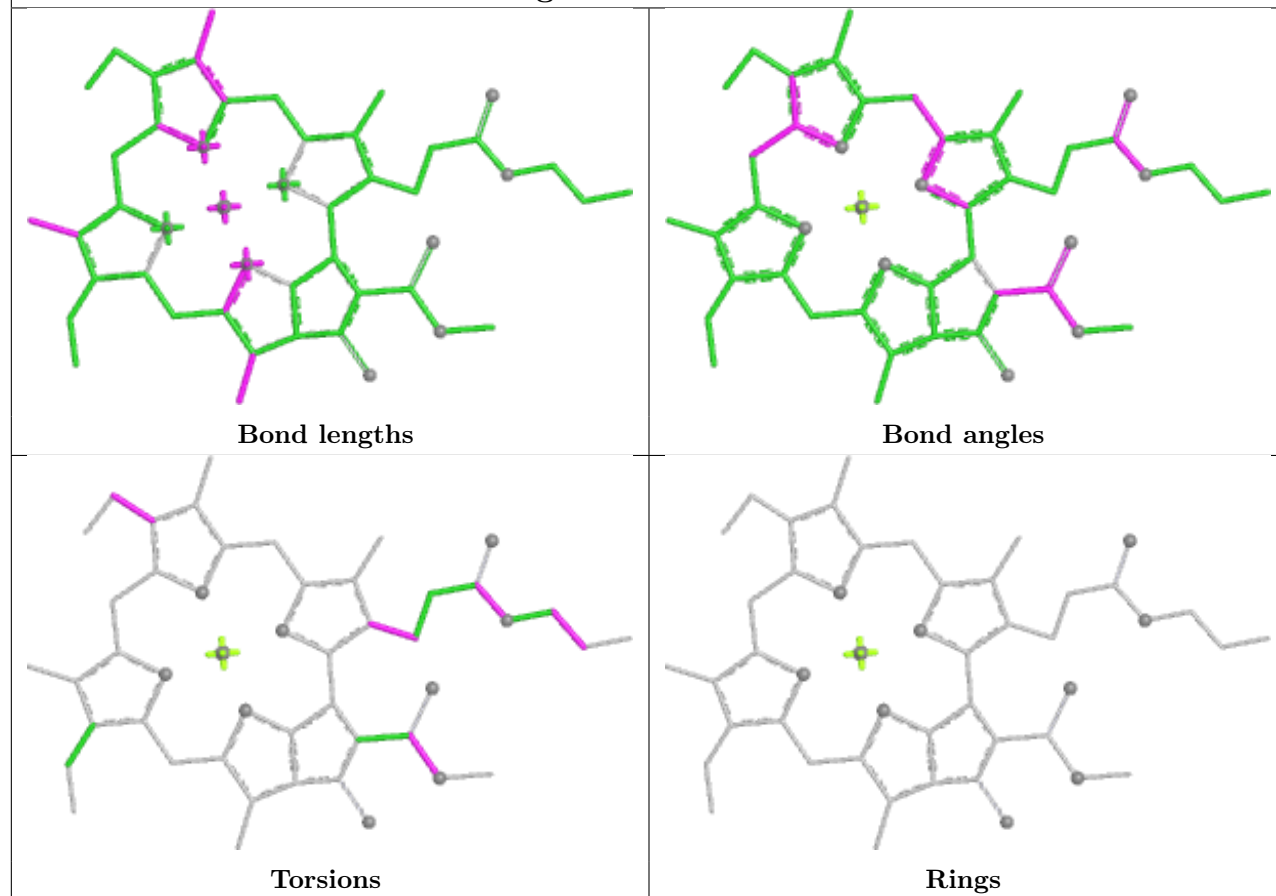


Torsions

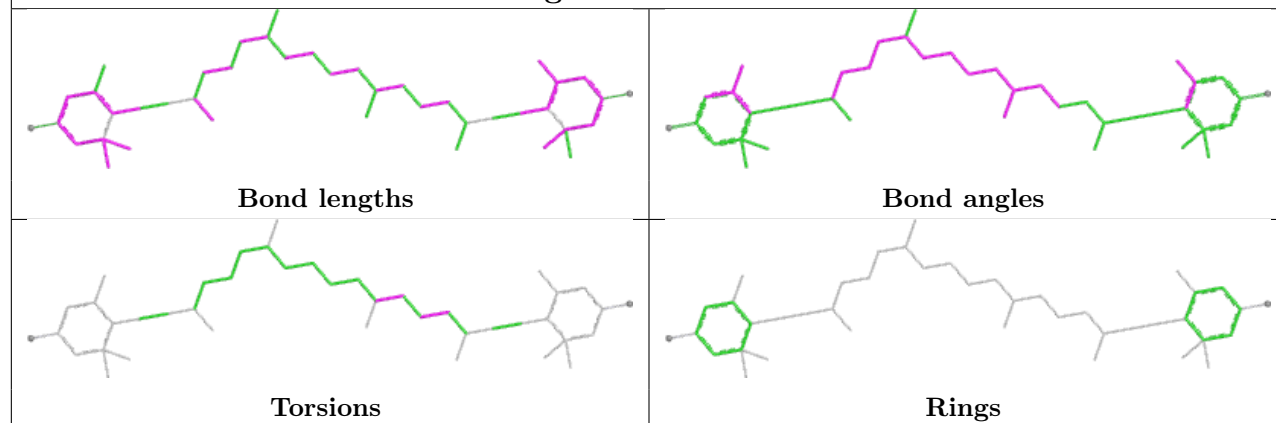


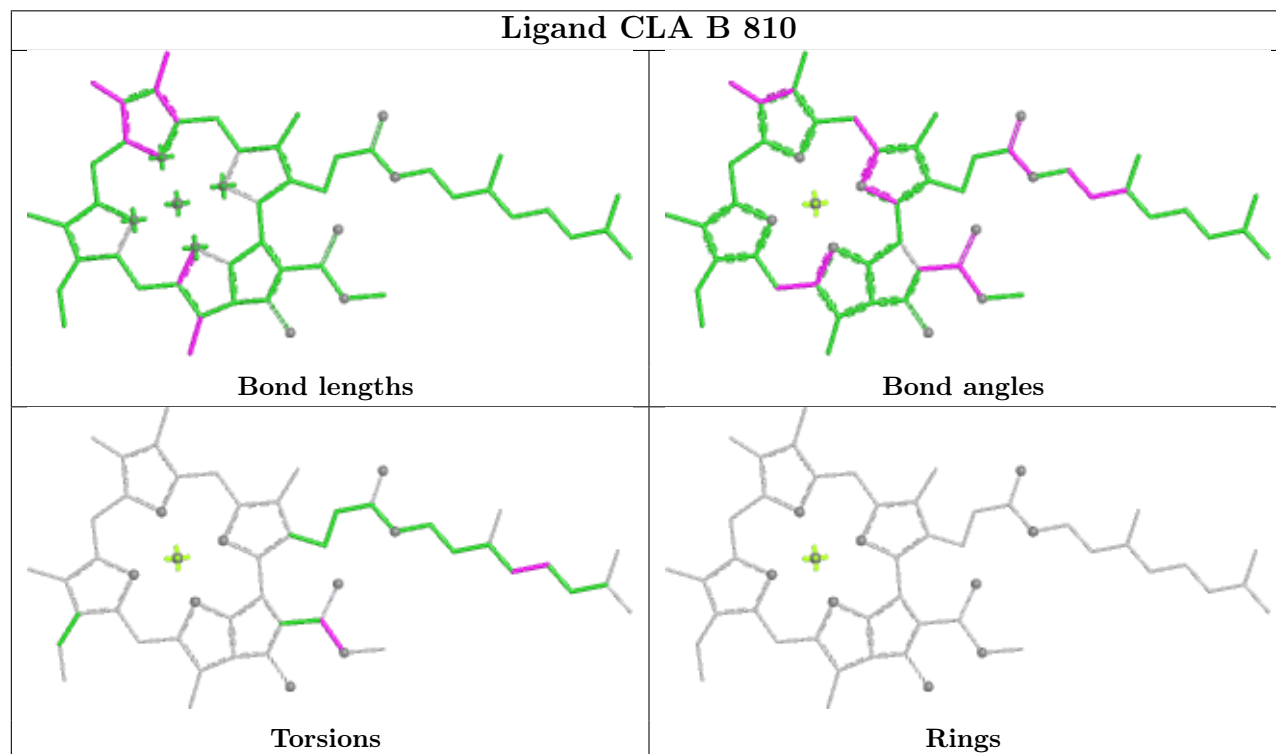
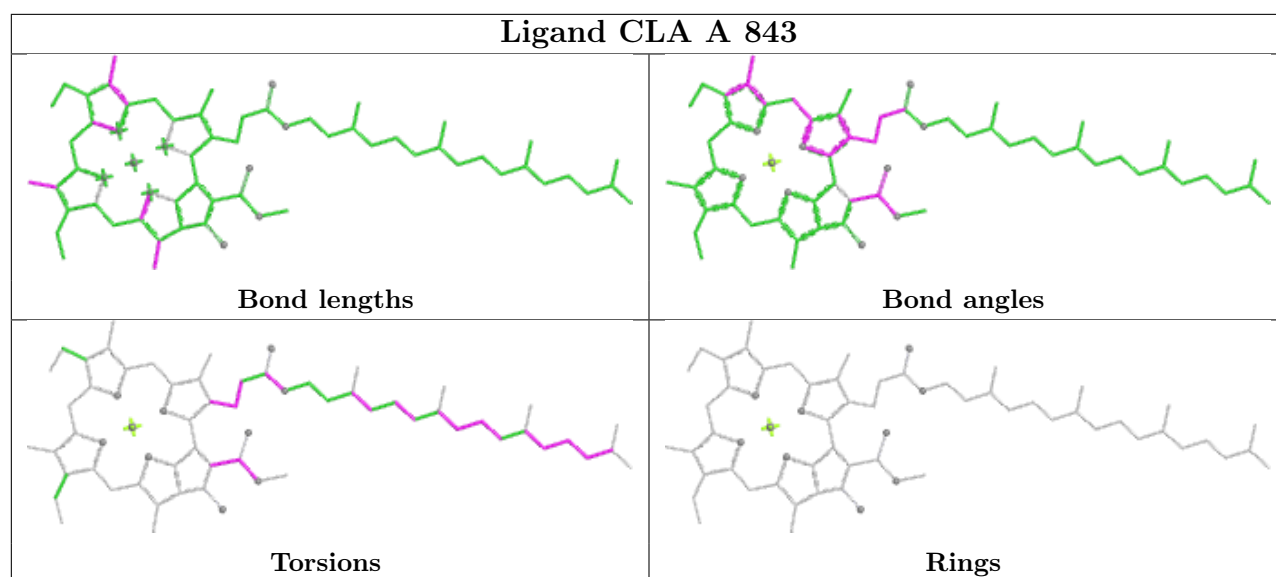
Rings

## Ligand CLA a 310

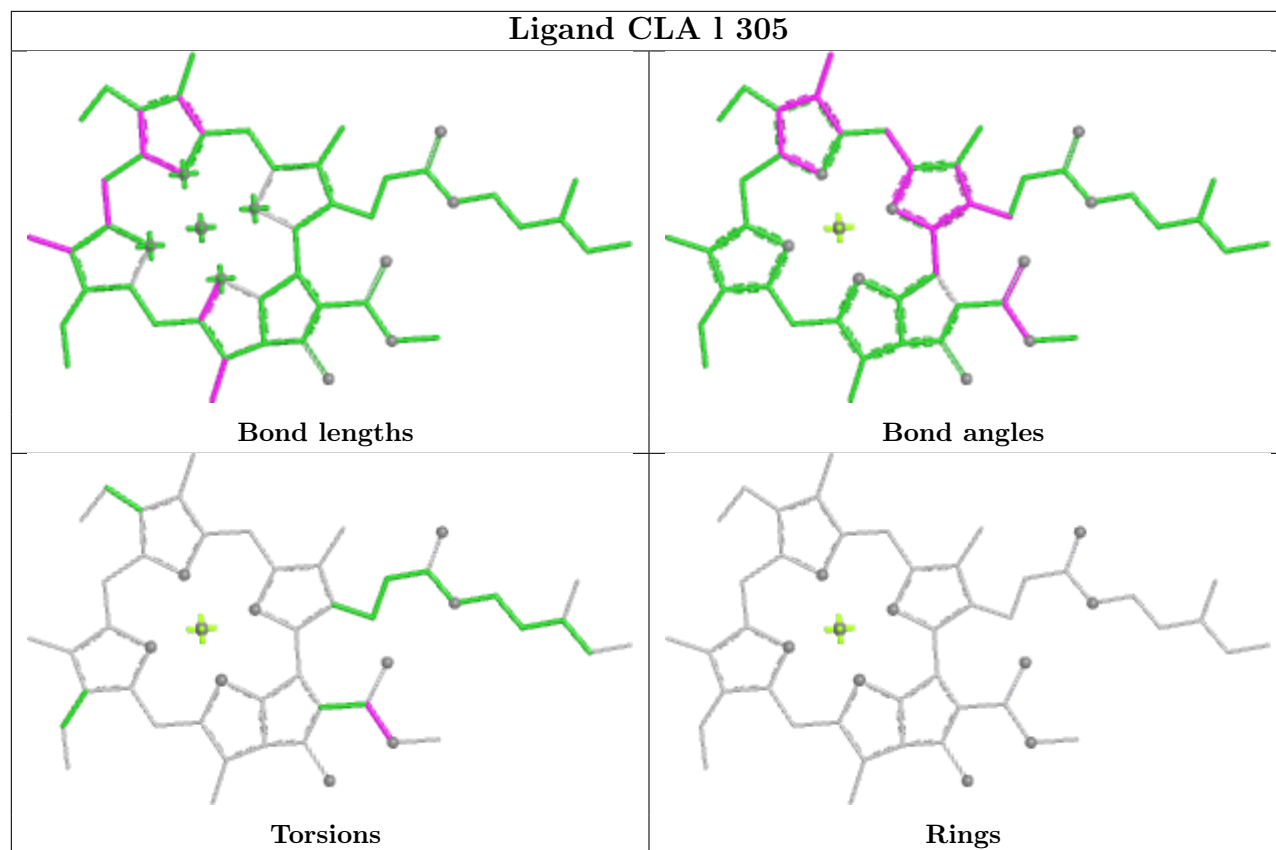


## Ligand II0 m 614

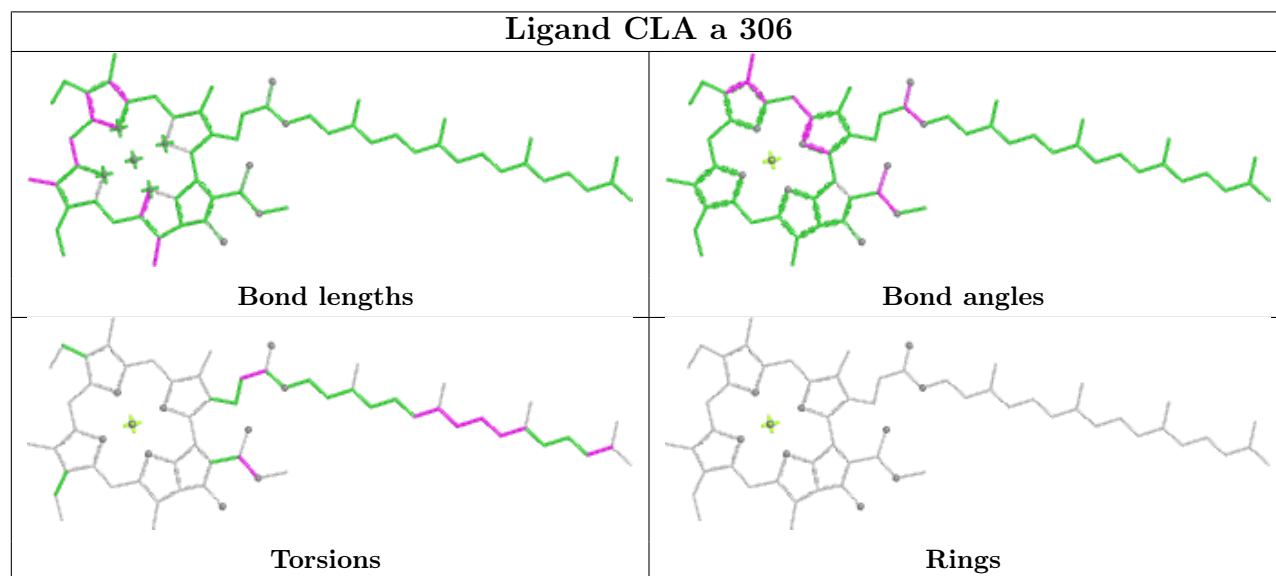




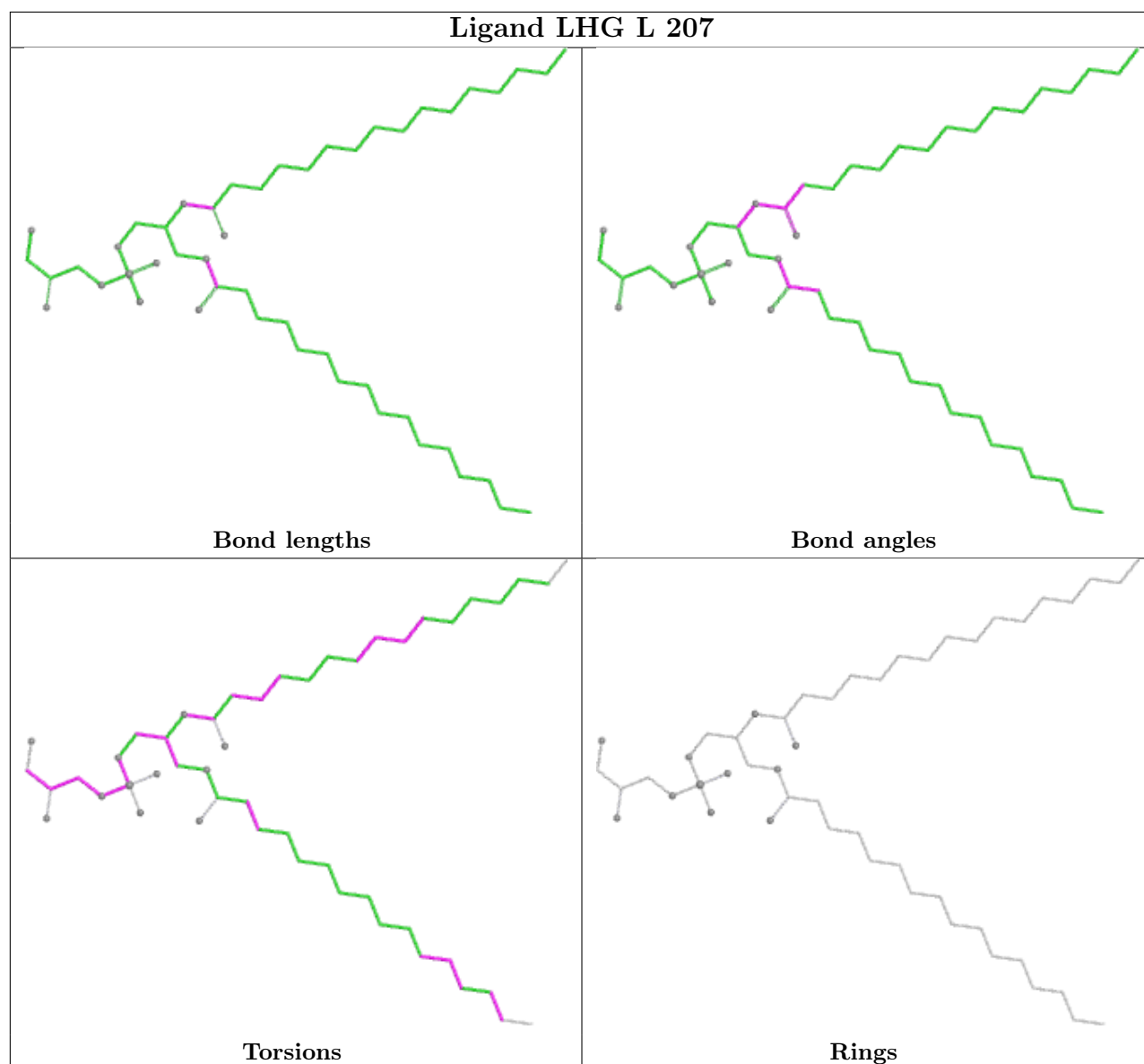
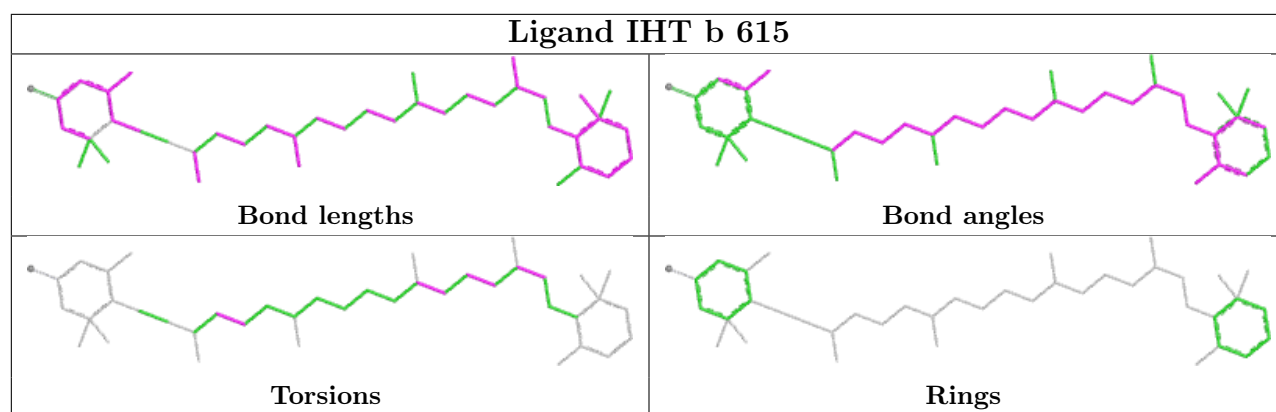
## Ligand CLA l 305

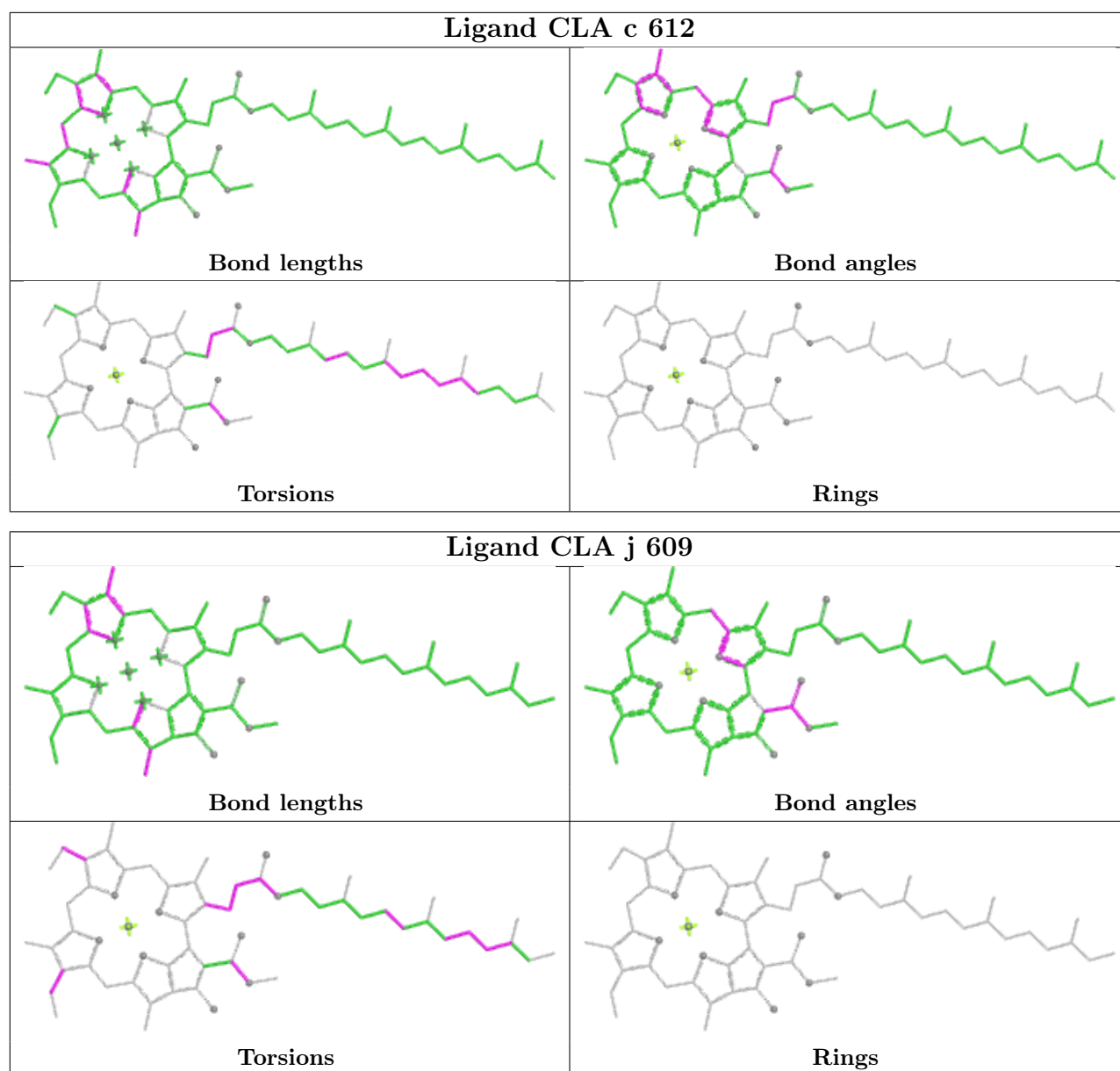


## Ligand CLA a 306

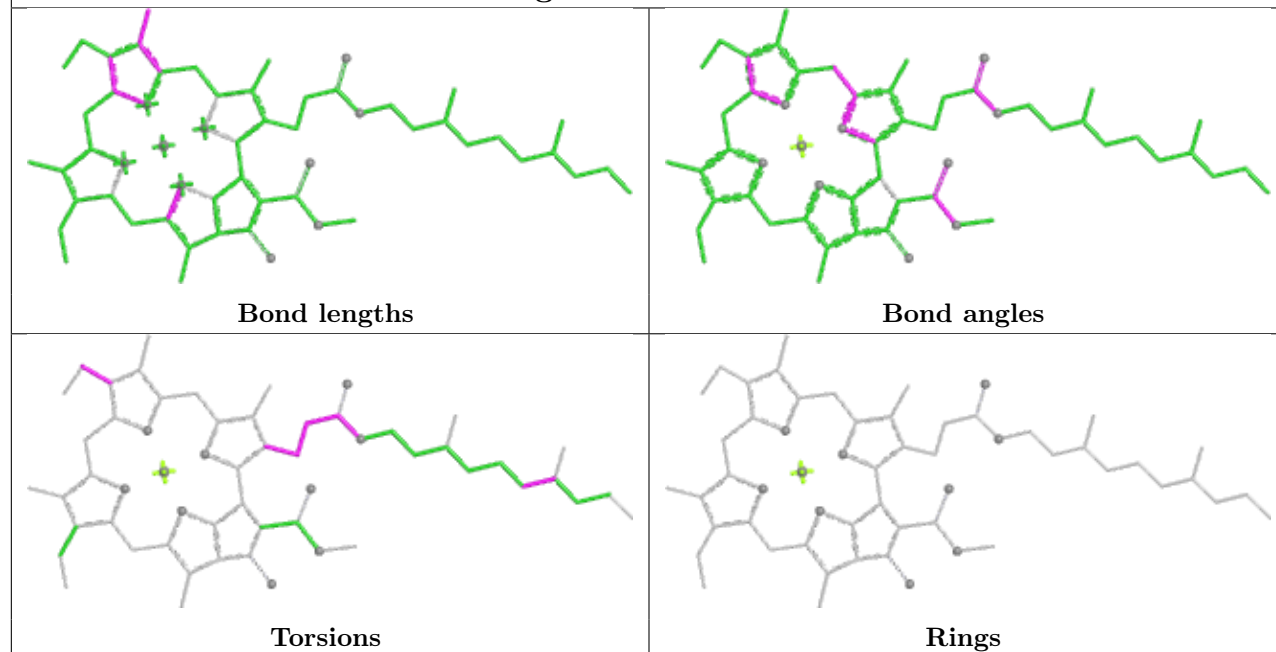




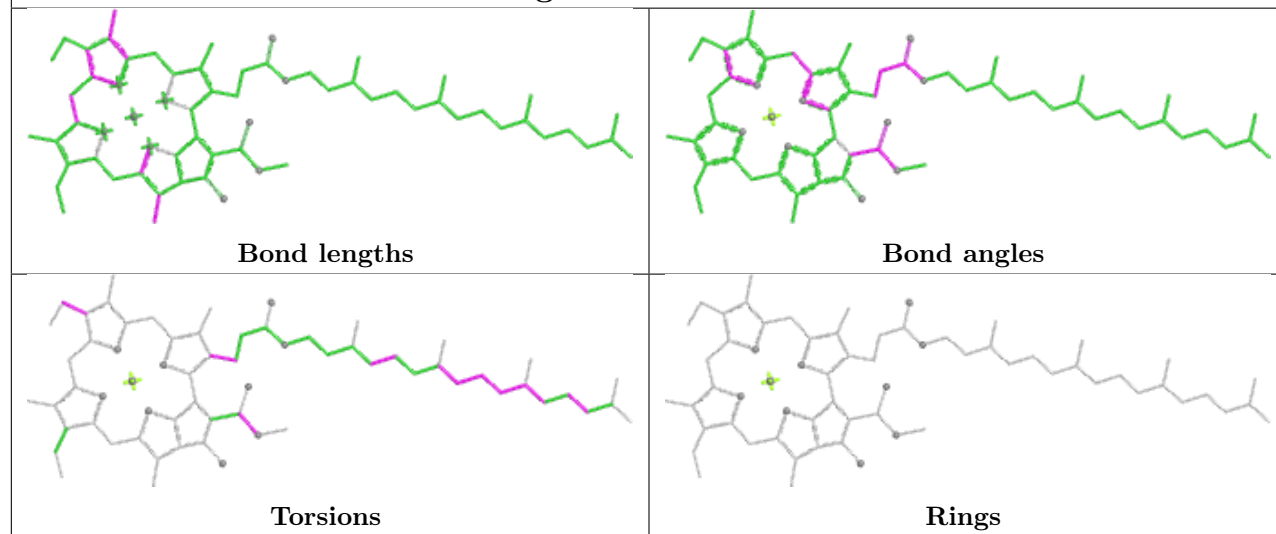


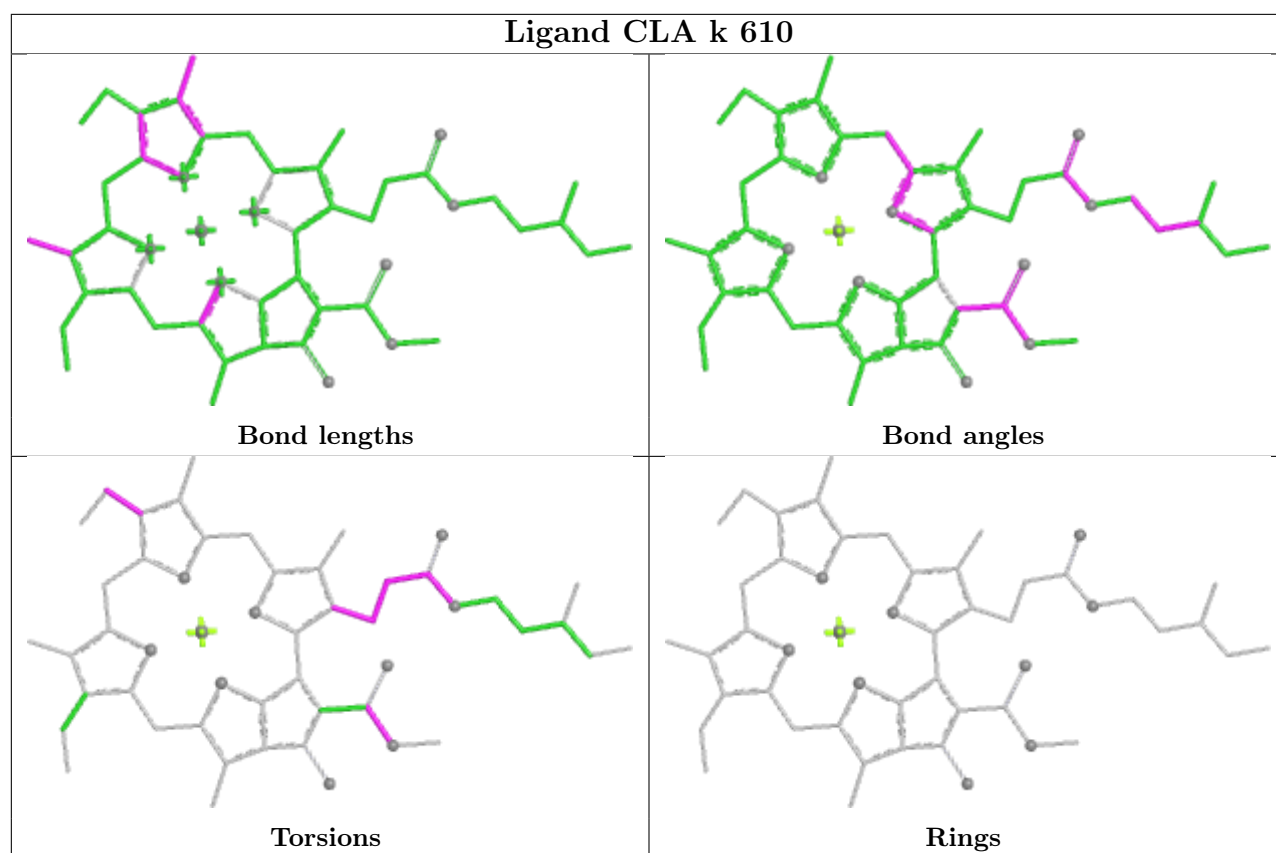


## Ligand CLA h 307

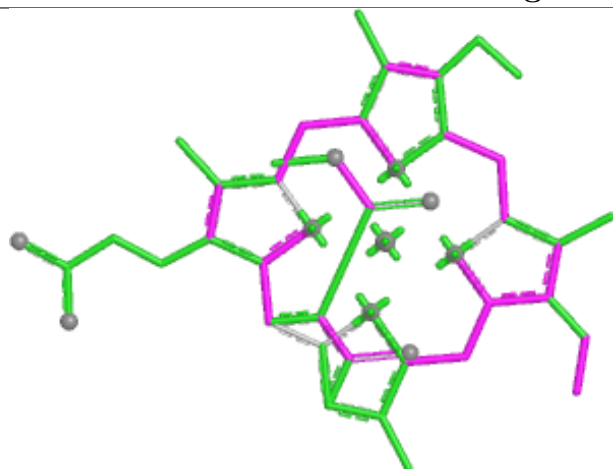


## Ligand CLA k 608

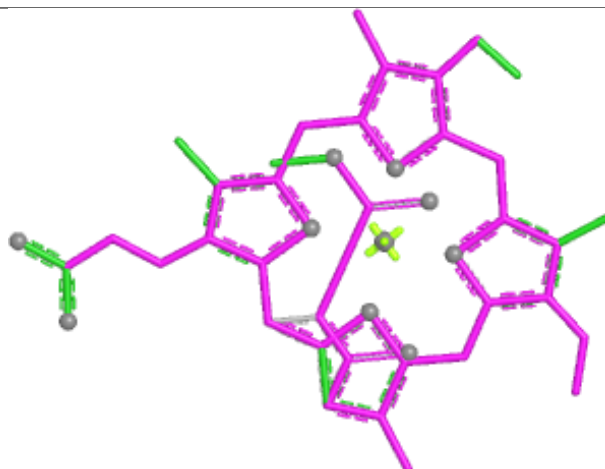




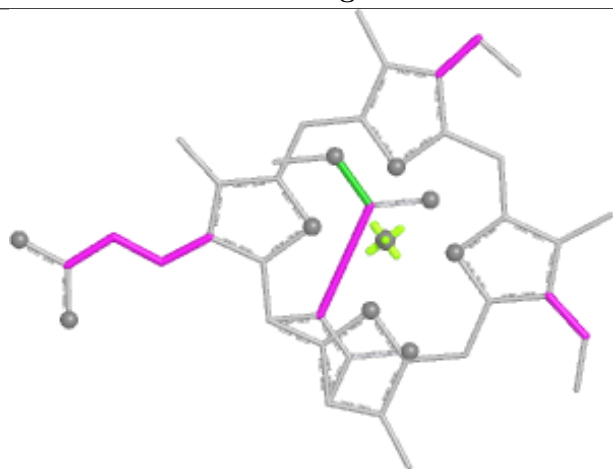
## Ligand KC2 I 311



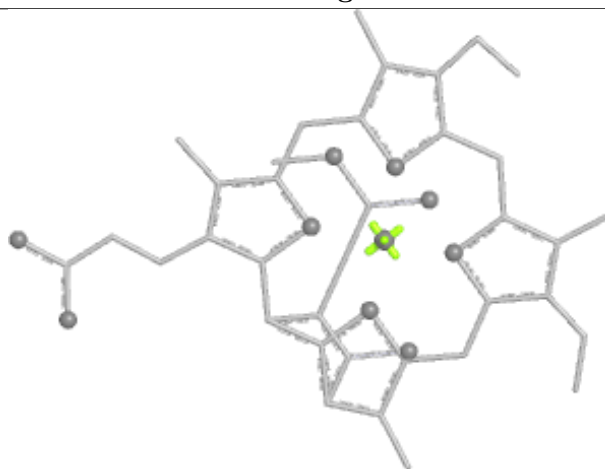
Bond lengths



Bond angles

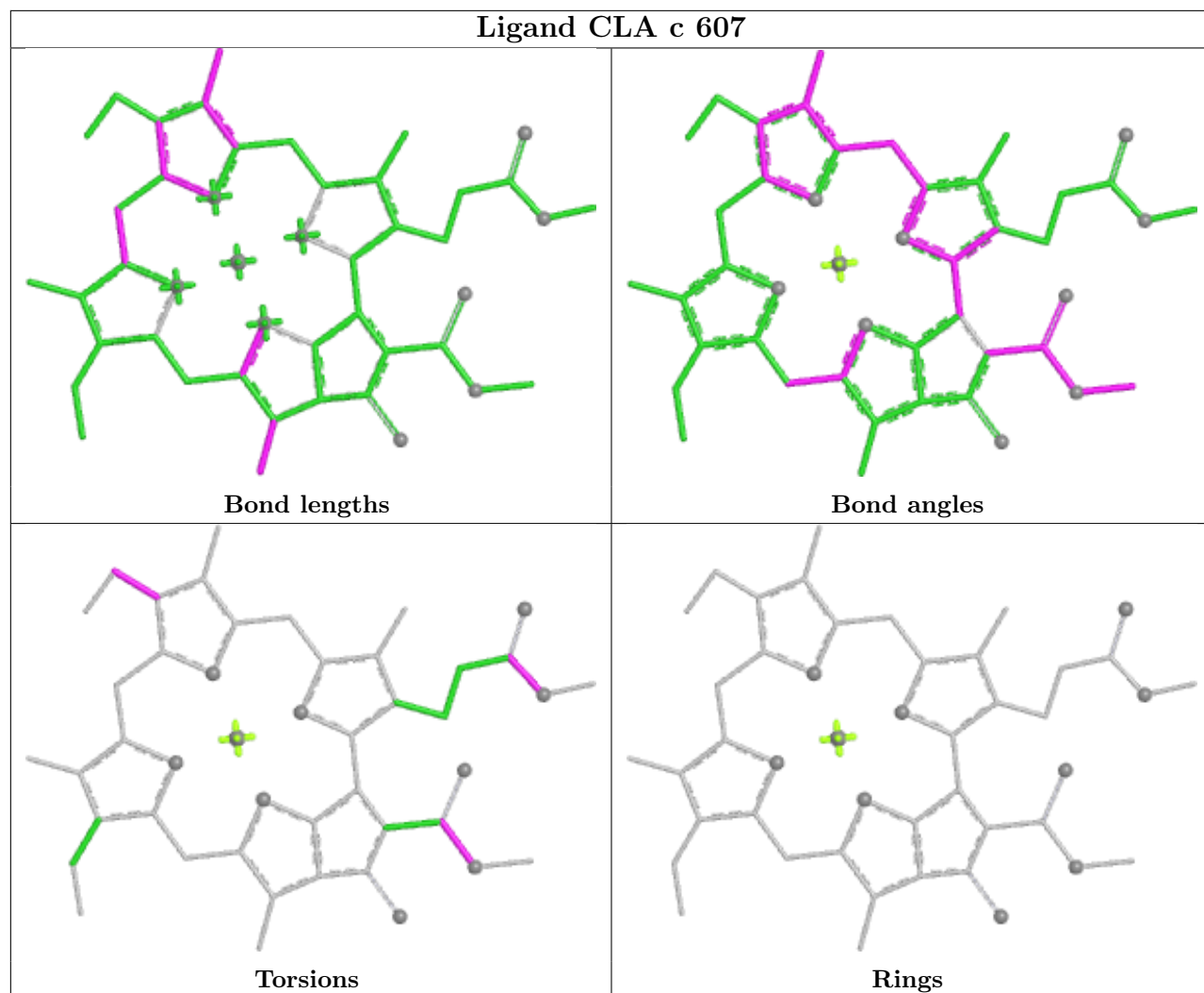


Torsions

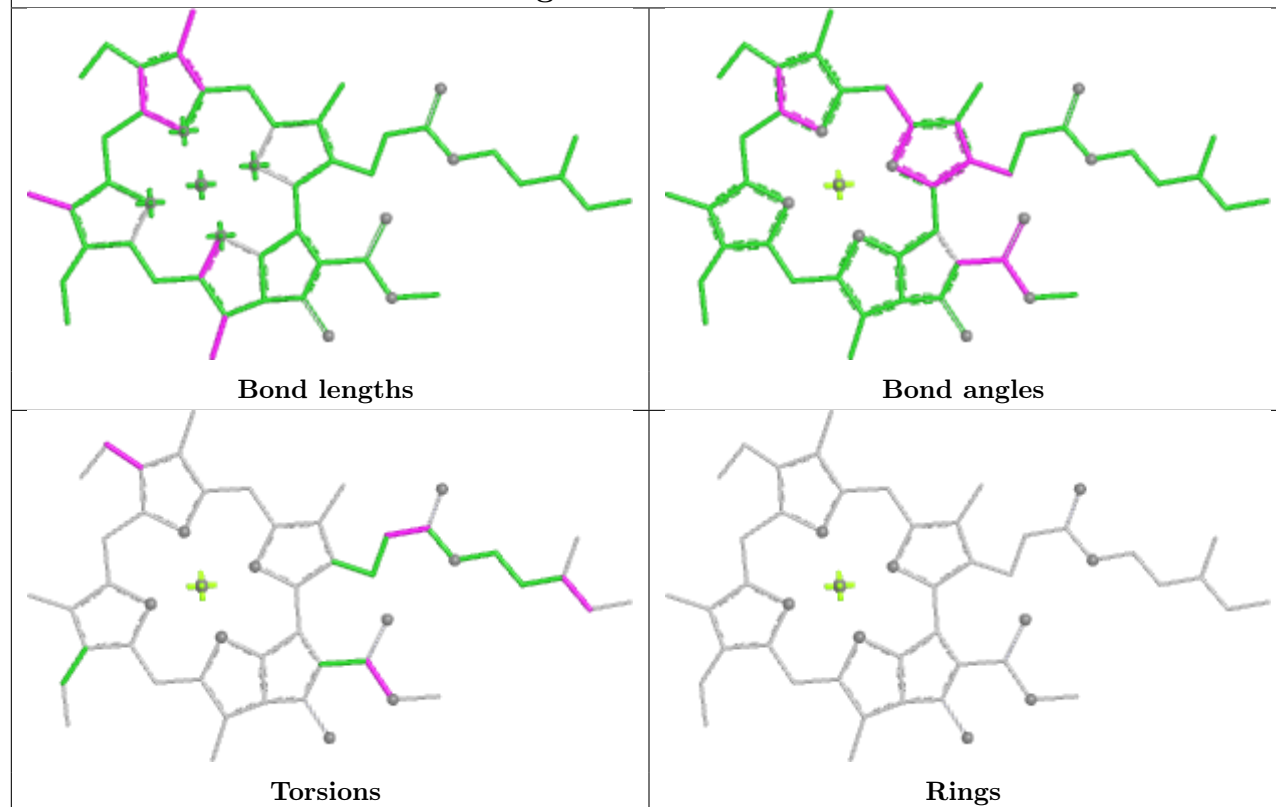


Rings

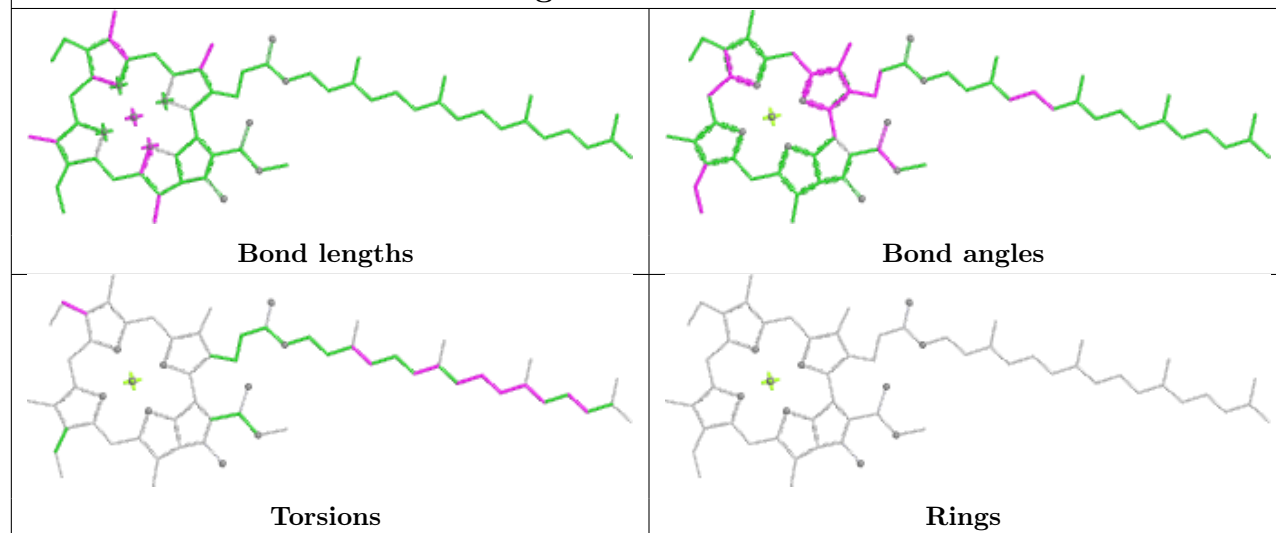
## Ligand CLA c 607



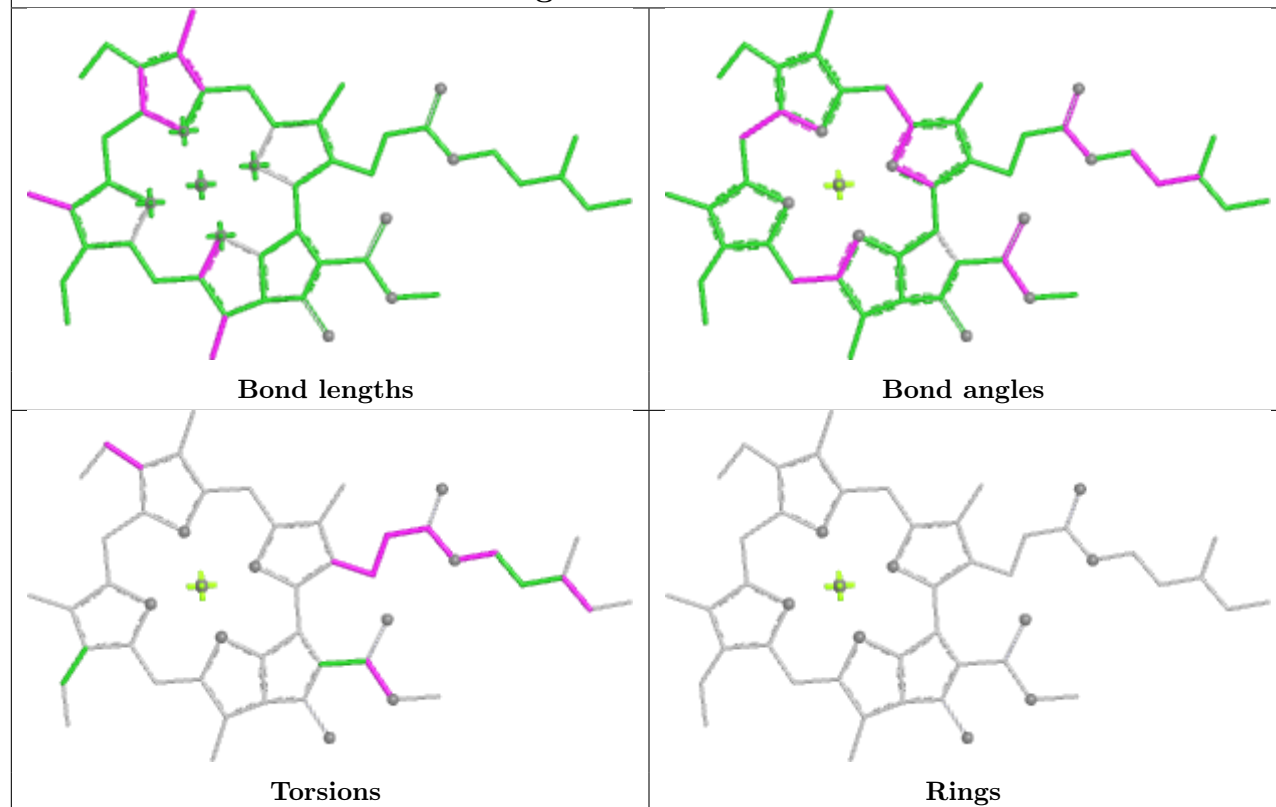
## Ligand CLA a 305



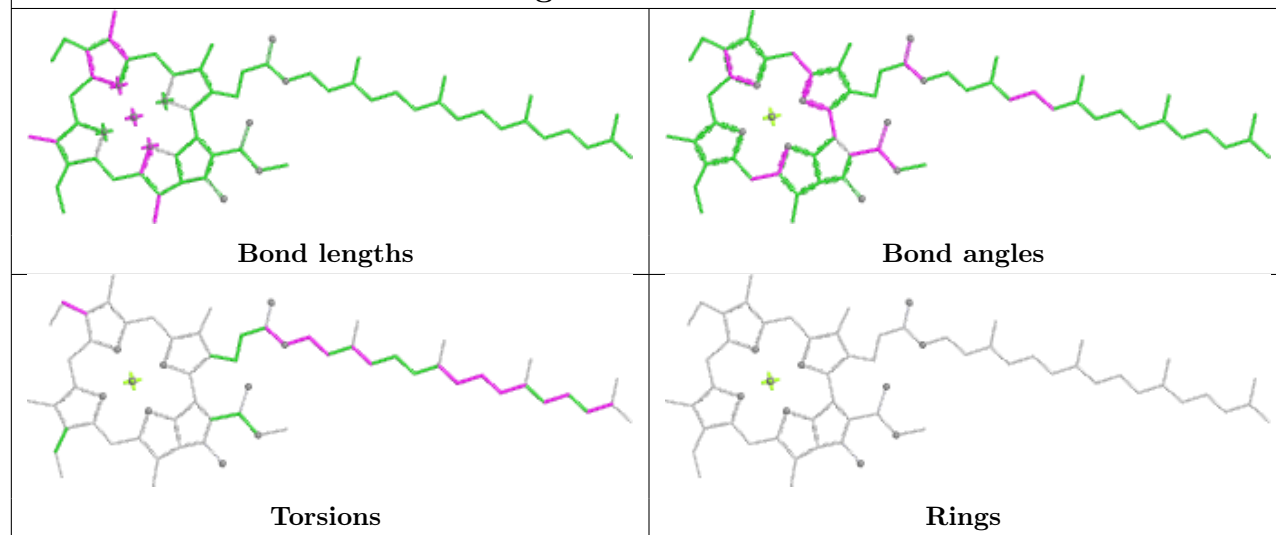
## Ligand CLA b 605



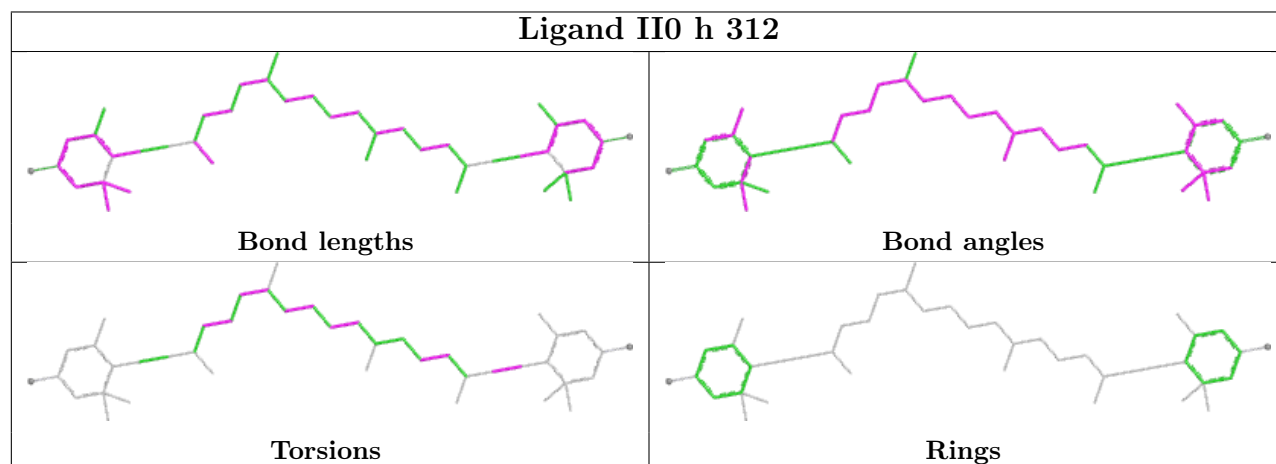
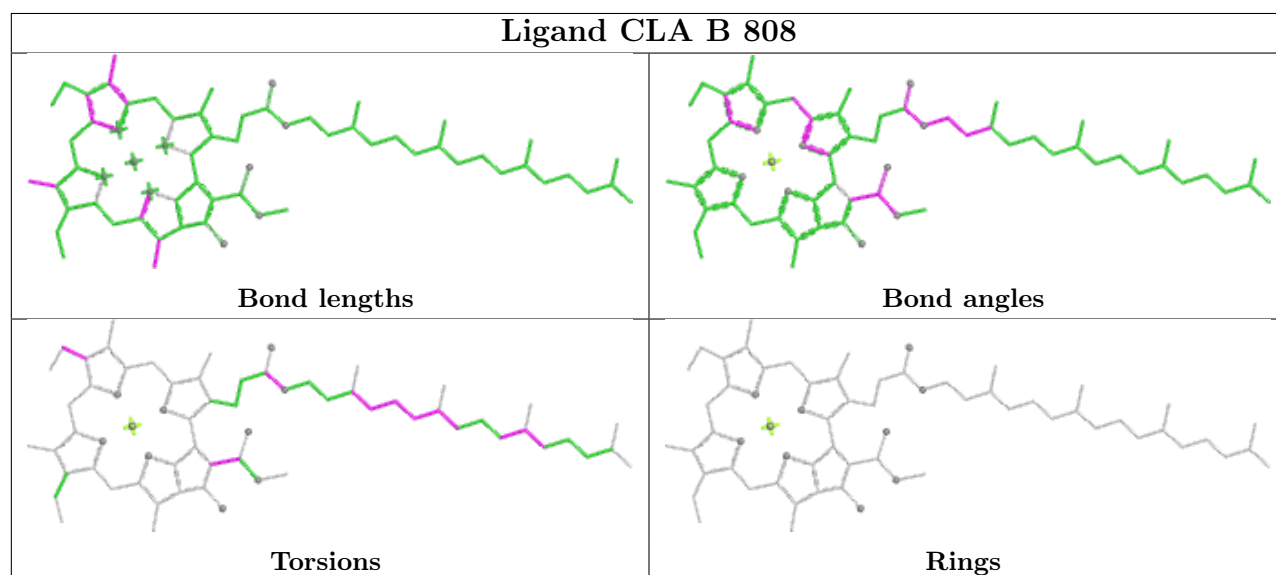
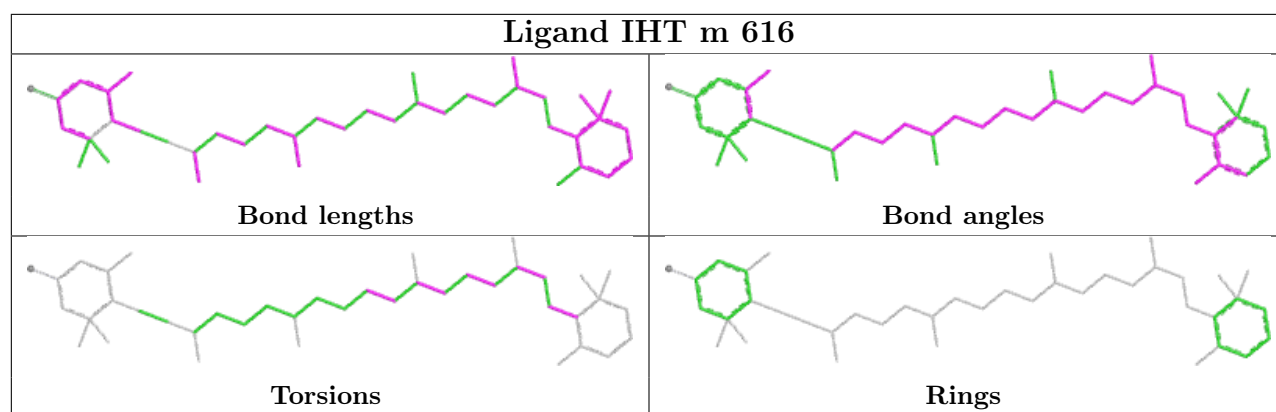
## Ligand CLA k 606

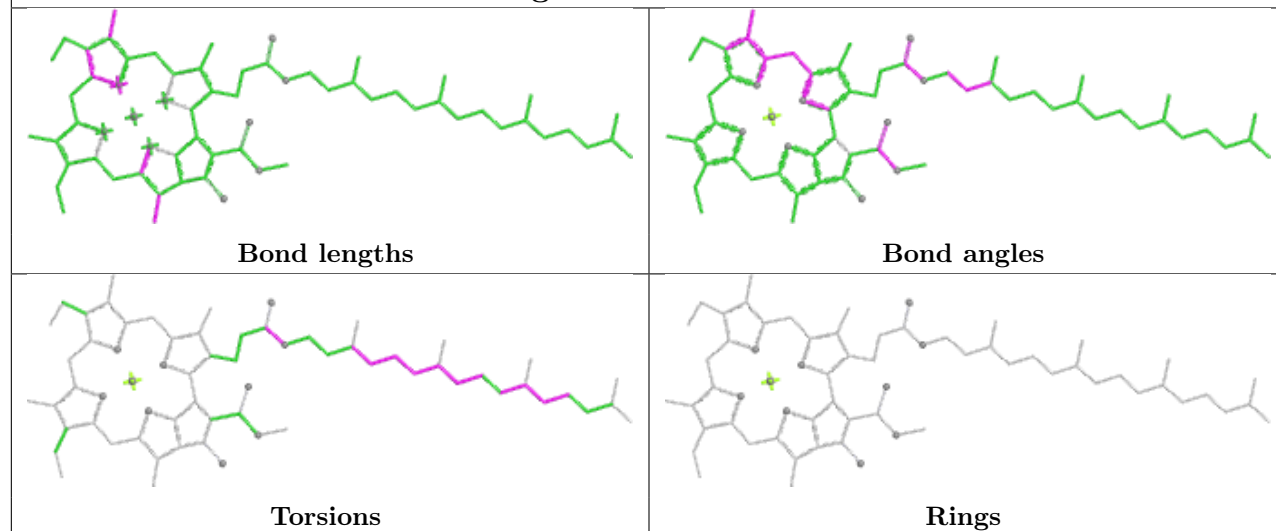
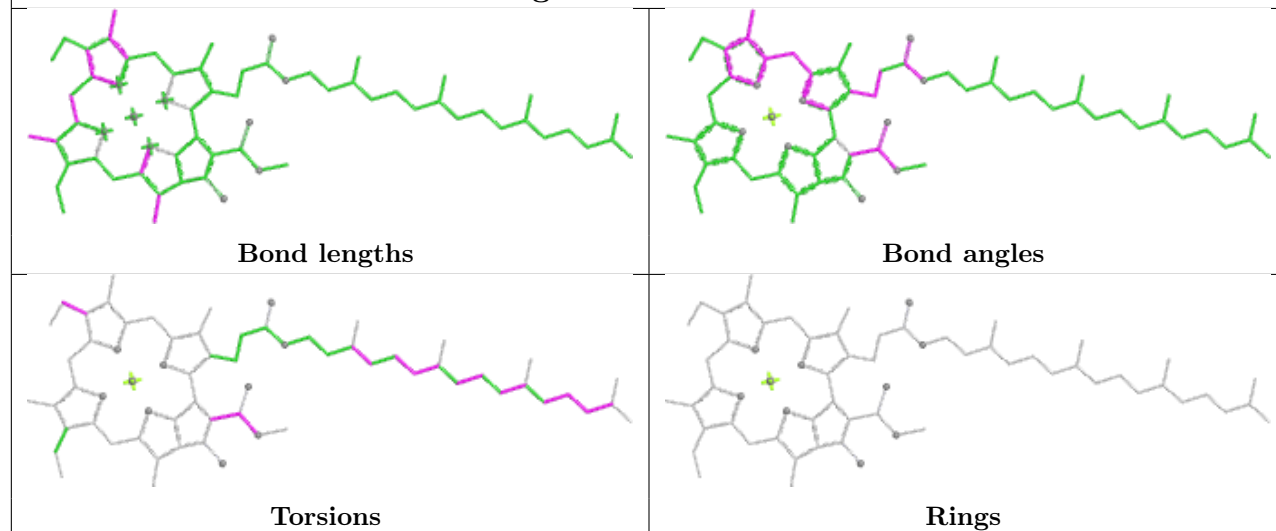


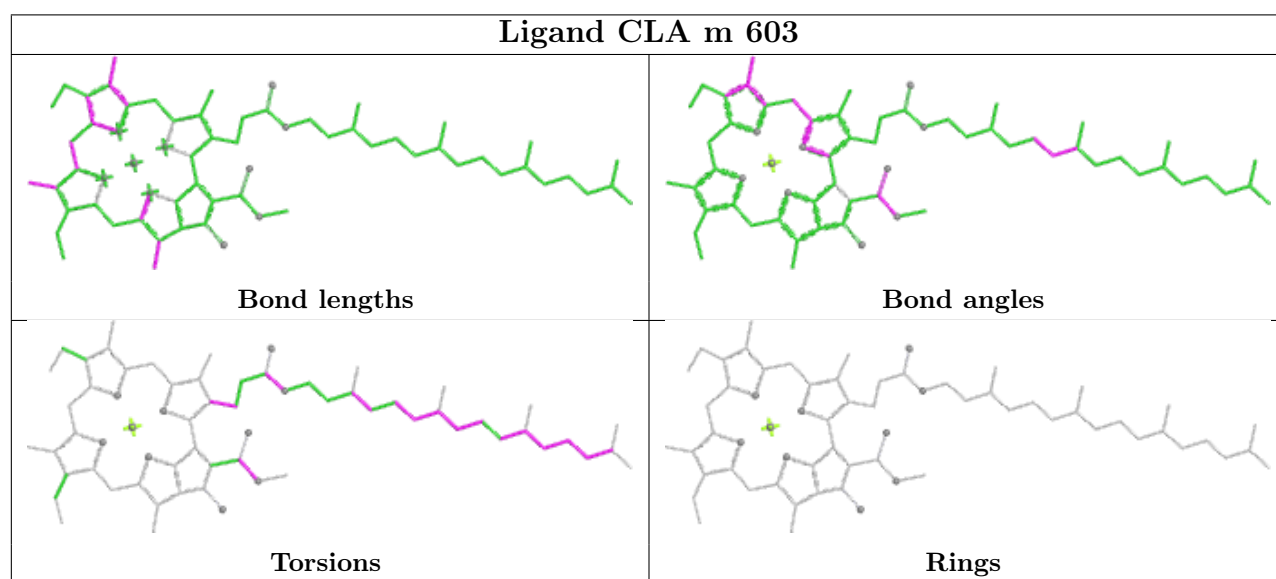
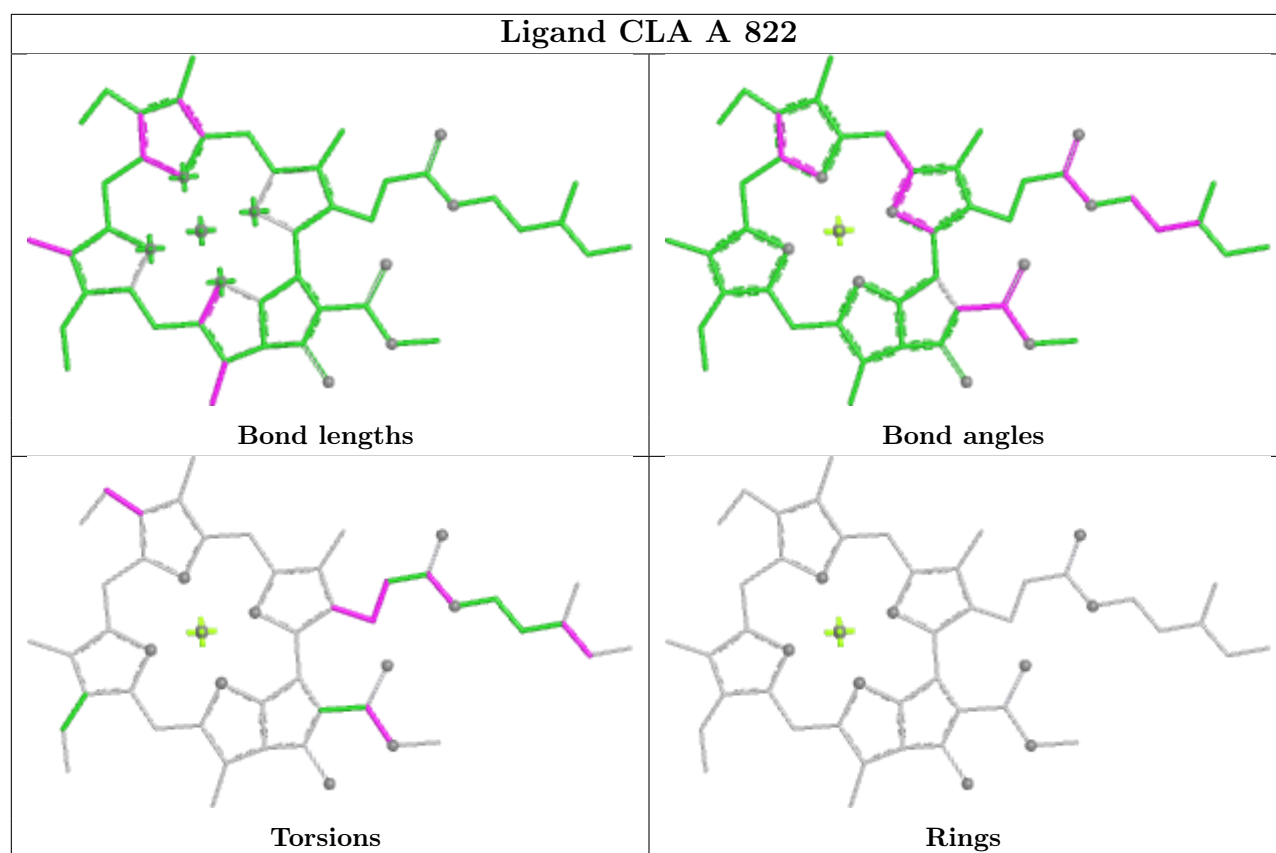
## Ligand CLA h 301



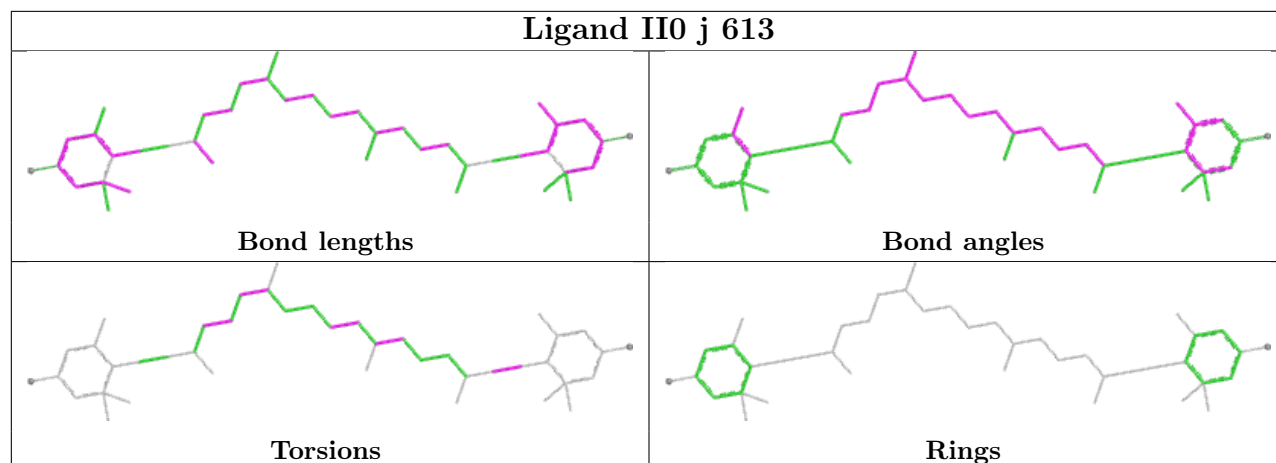




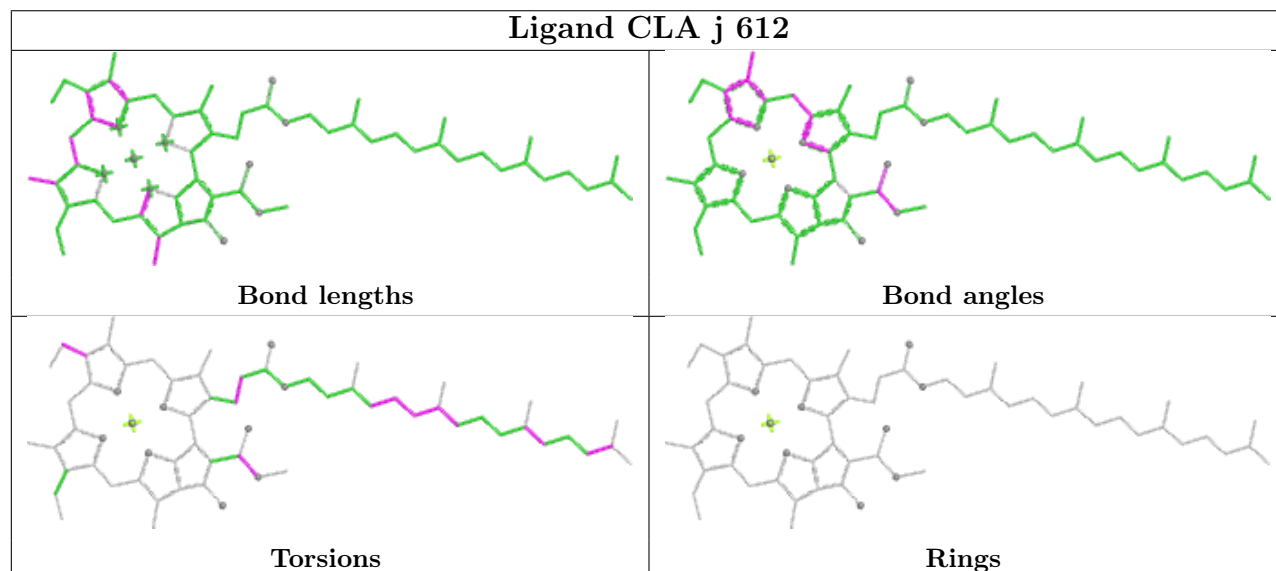
**Ligand CLA A 840****Ligand CLA B 833**



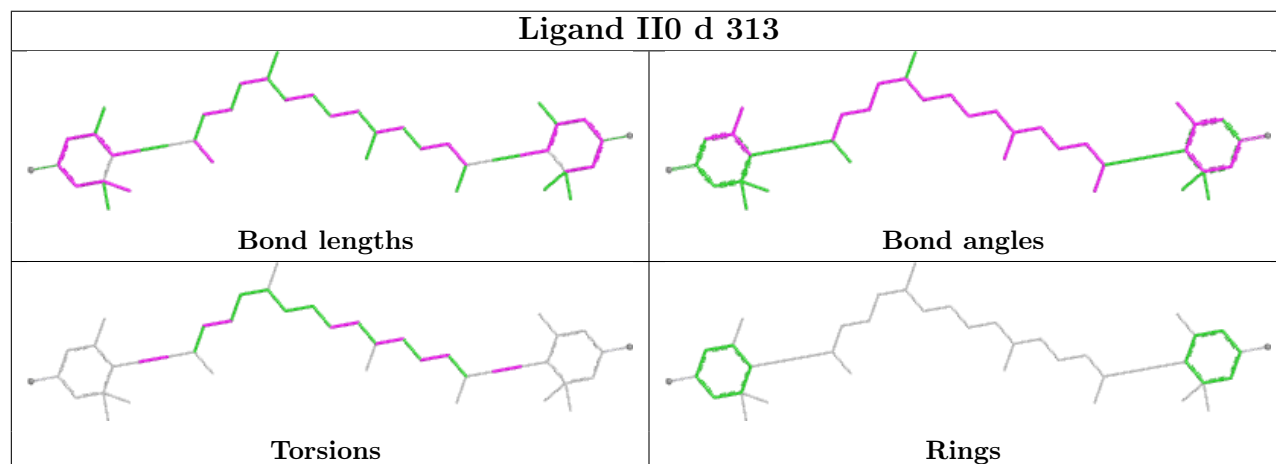
## Ligand II0 j 613



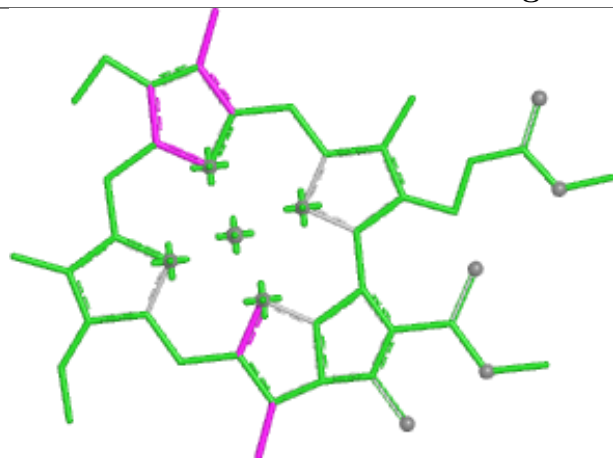
## Ligand CLA j 612



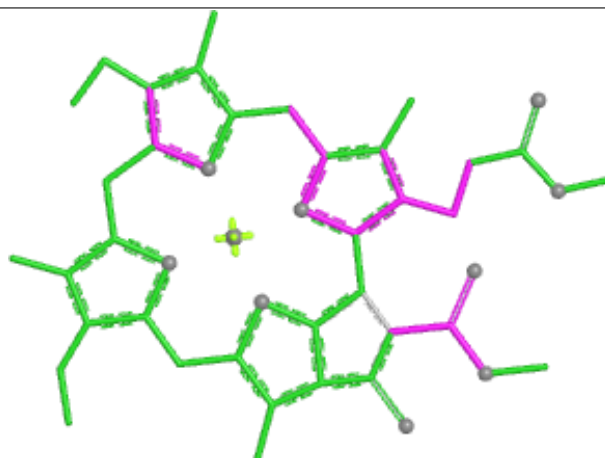
## Ligand II0 d 313



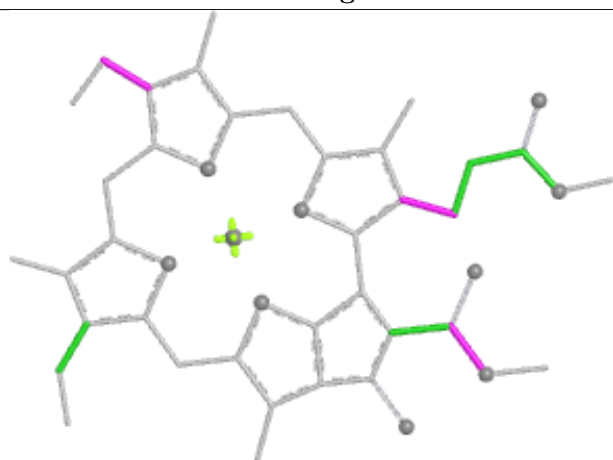
## Ligand CLA i 309



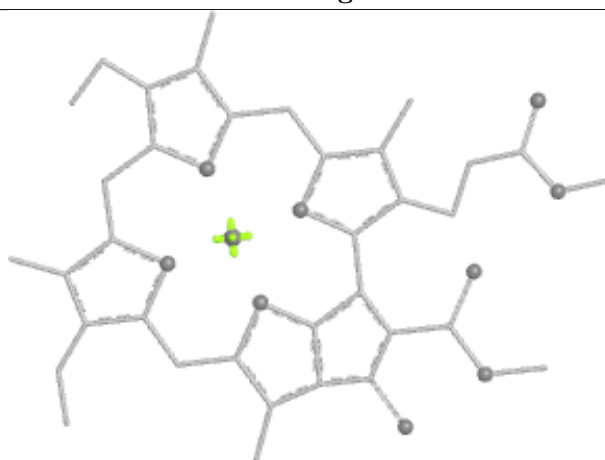
Bond lengths



Bond angles

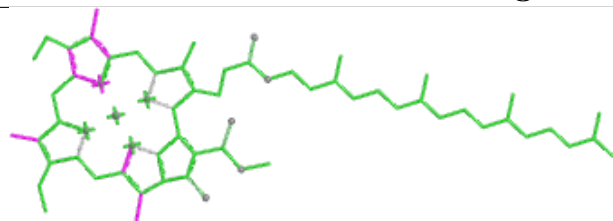


Torsions

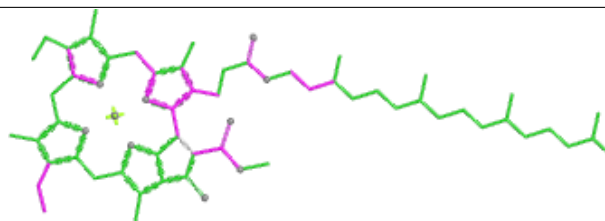


Rings

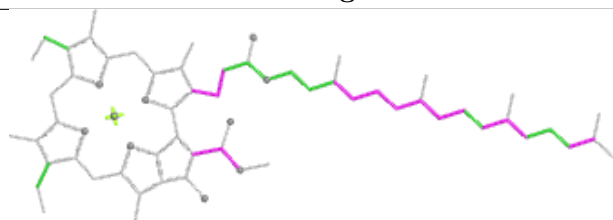
## Ligand CLA B 812



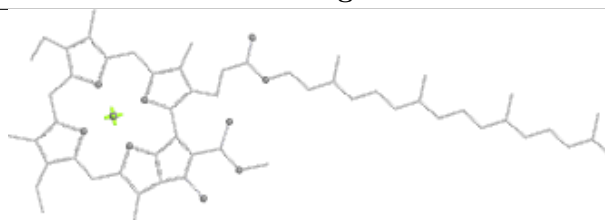
Bond lengths



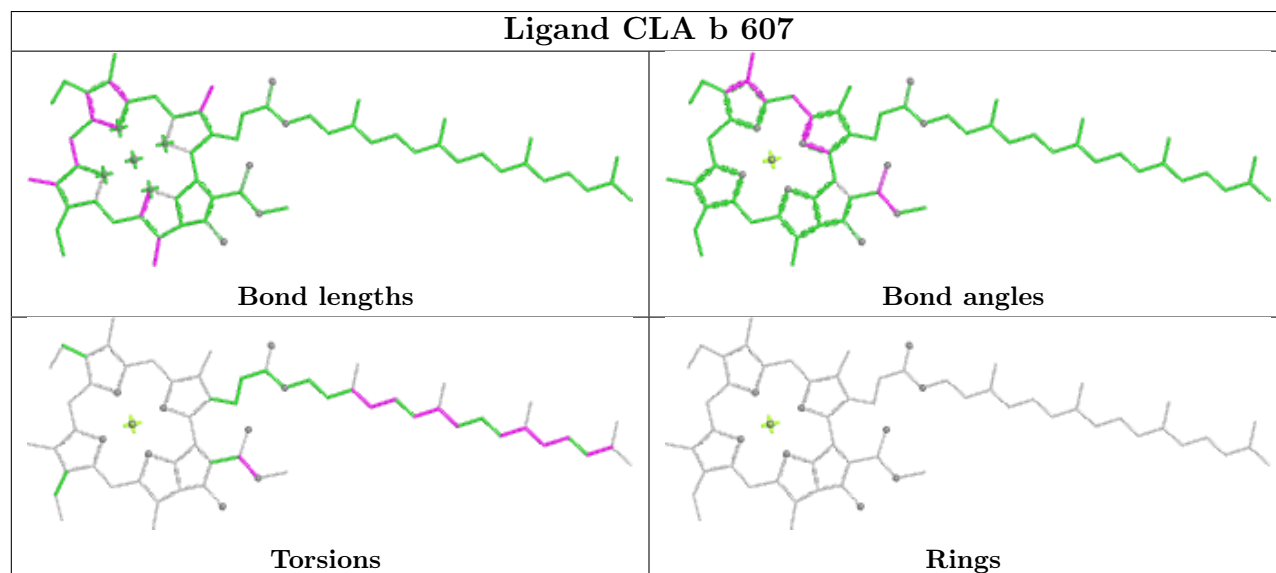
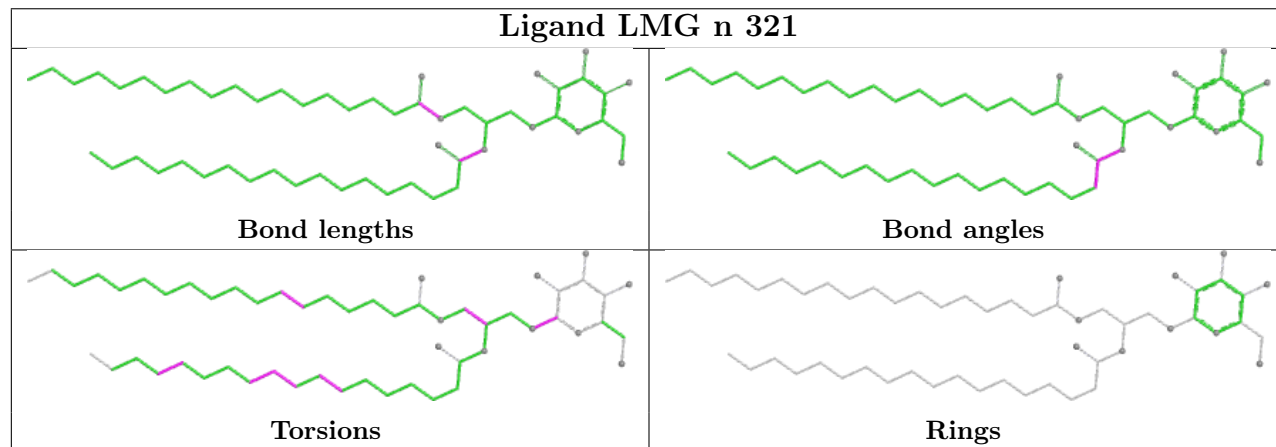
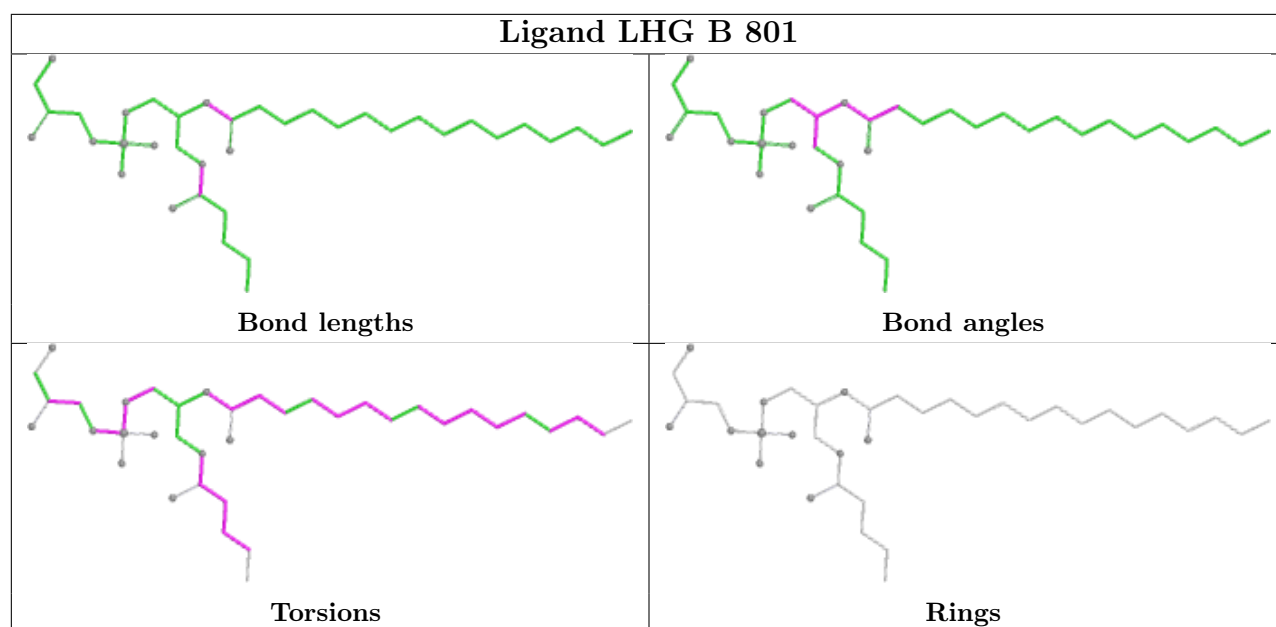
Bond angles

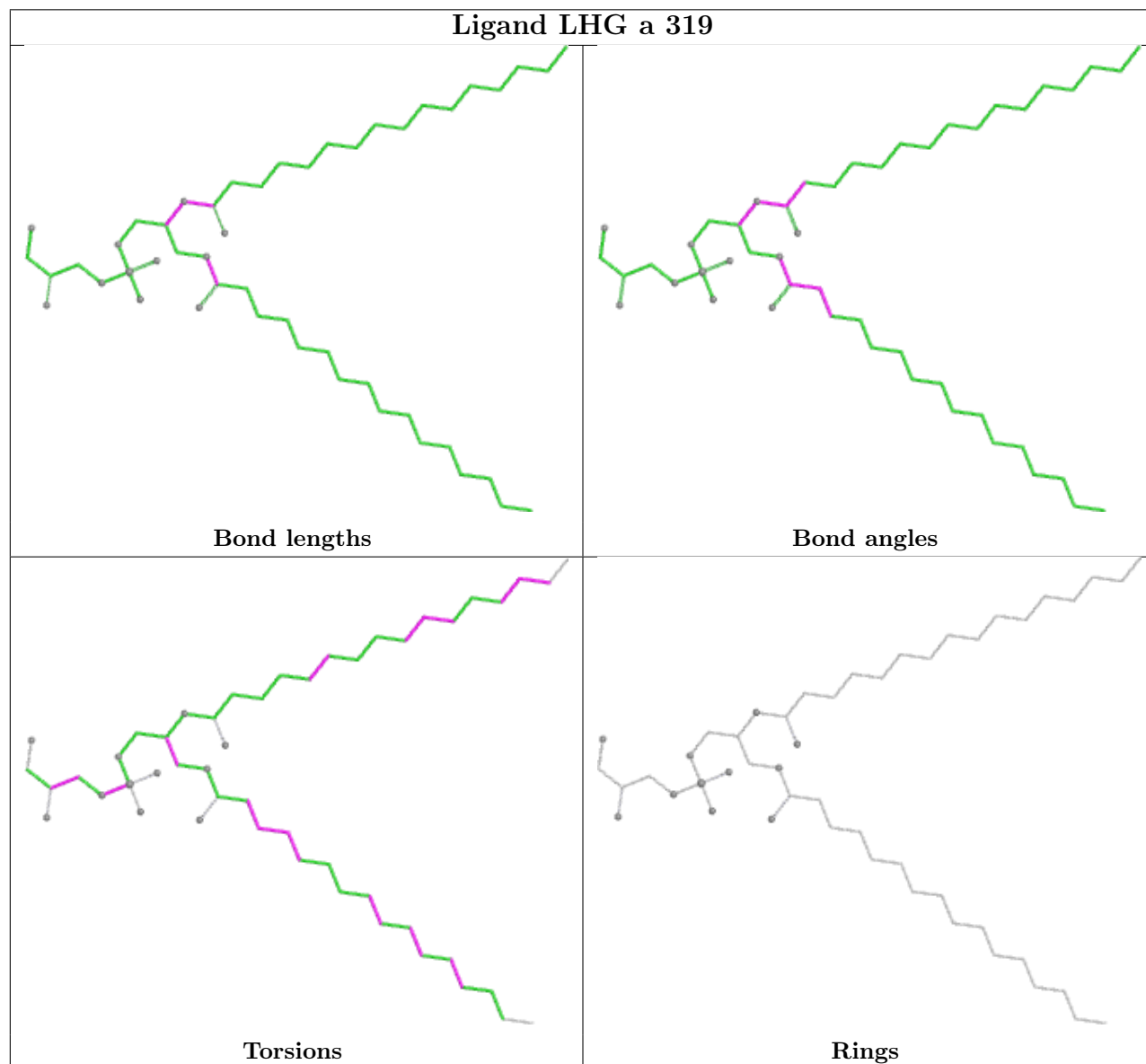
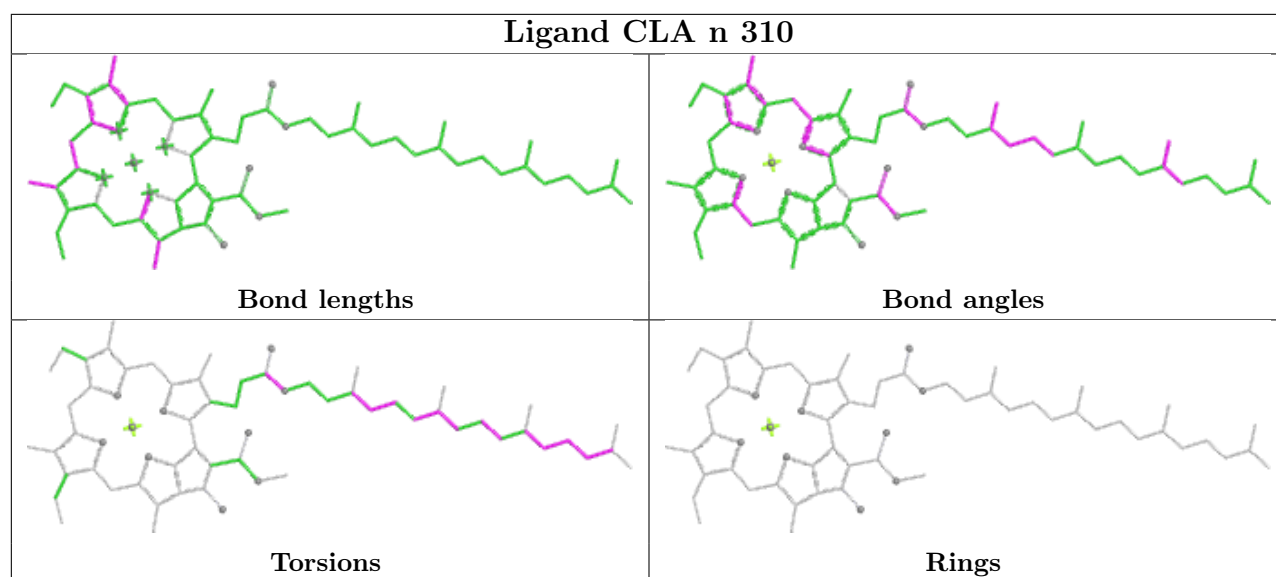


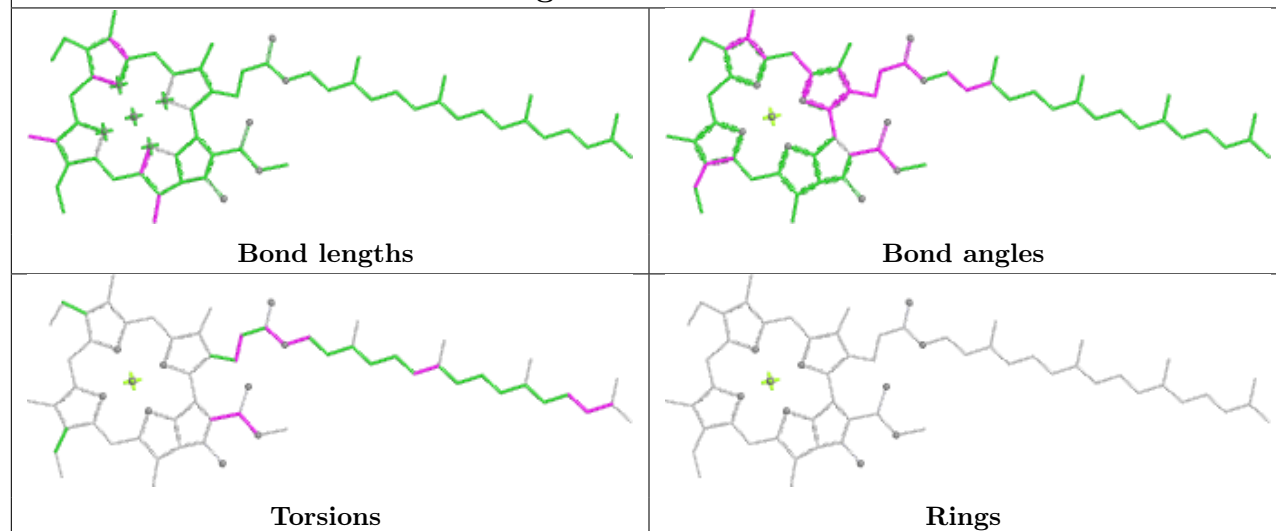
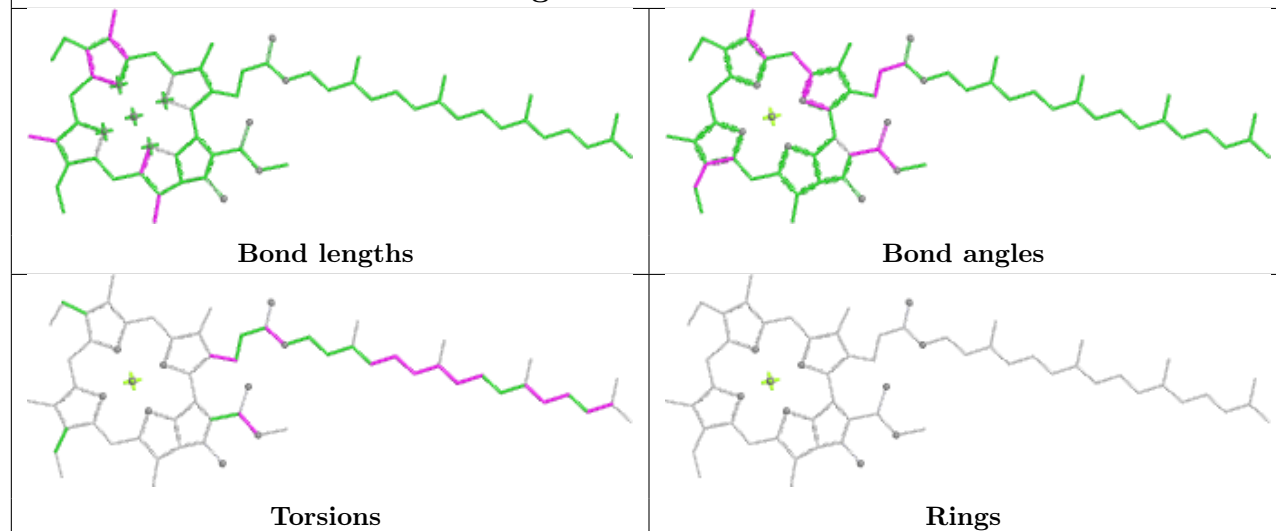
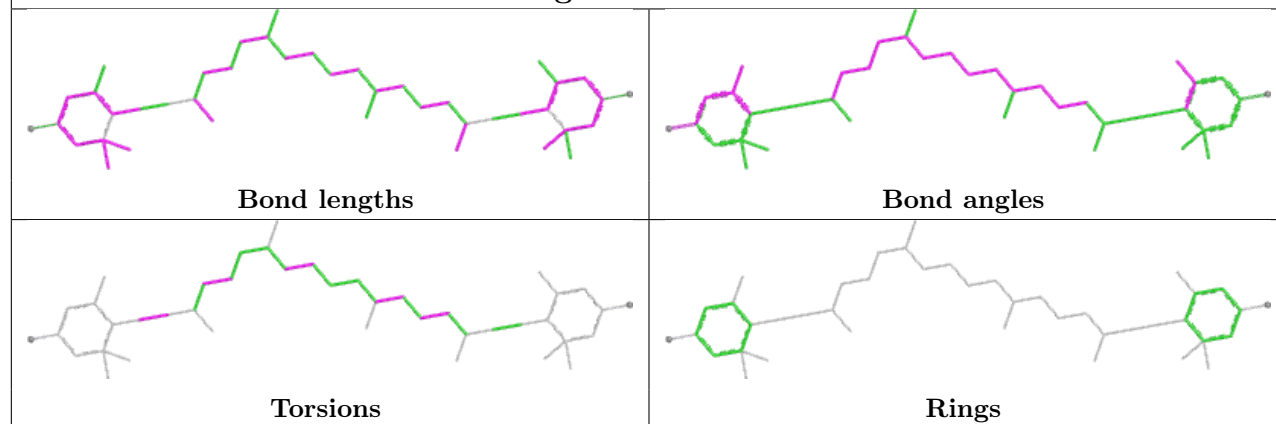
Torsions



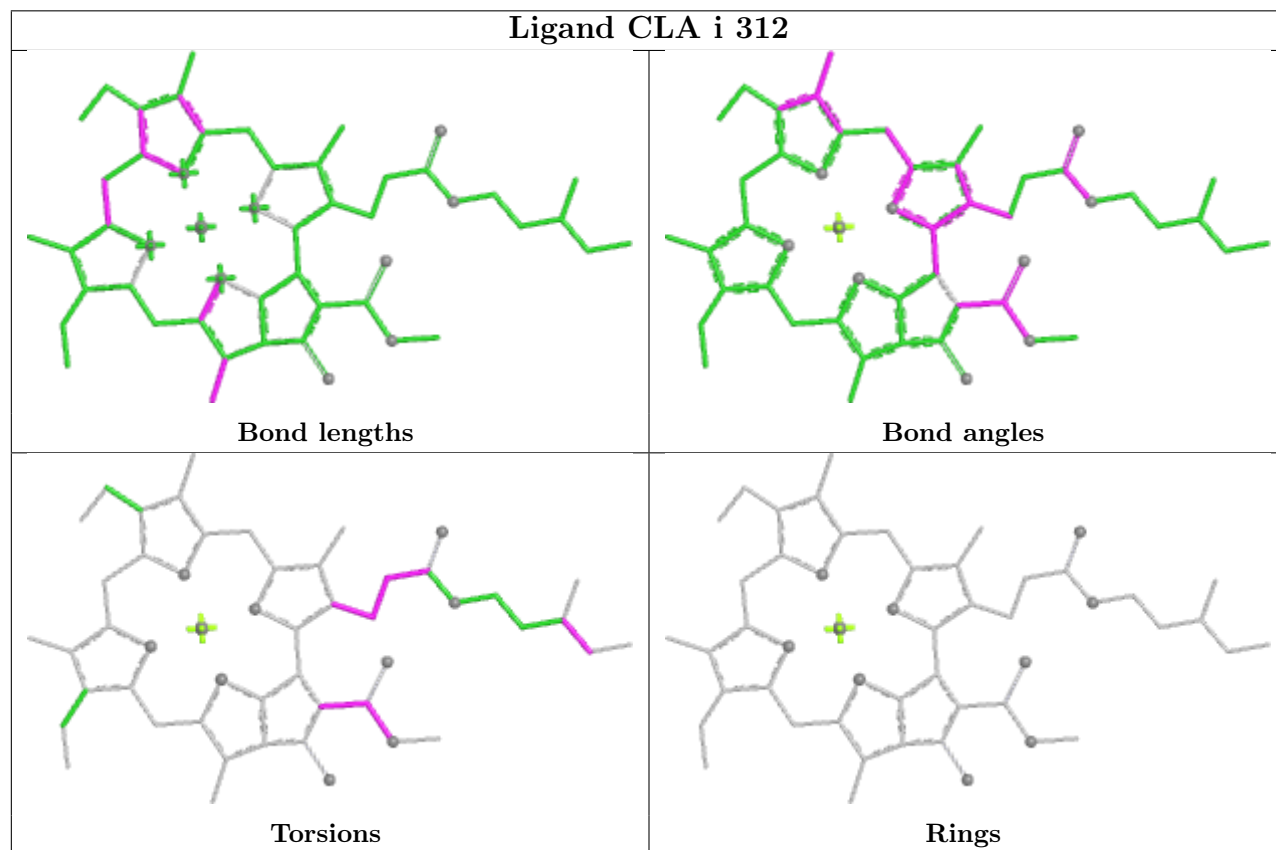
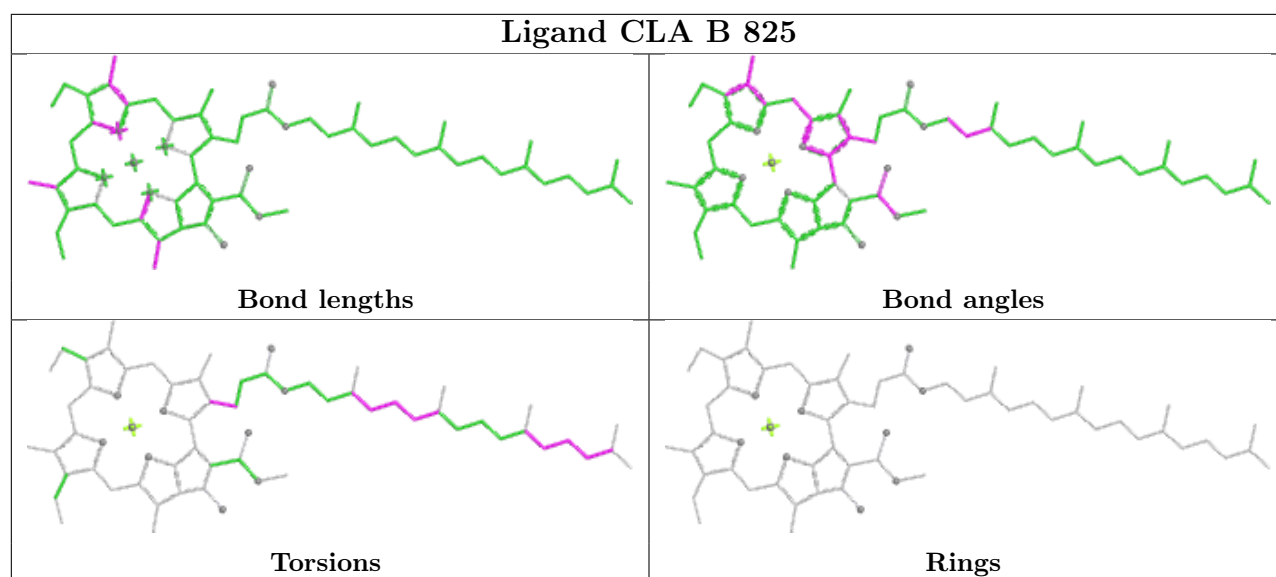
Rings

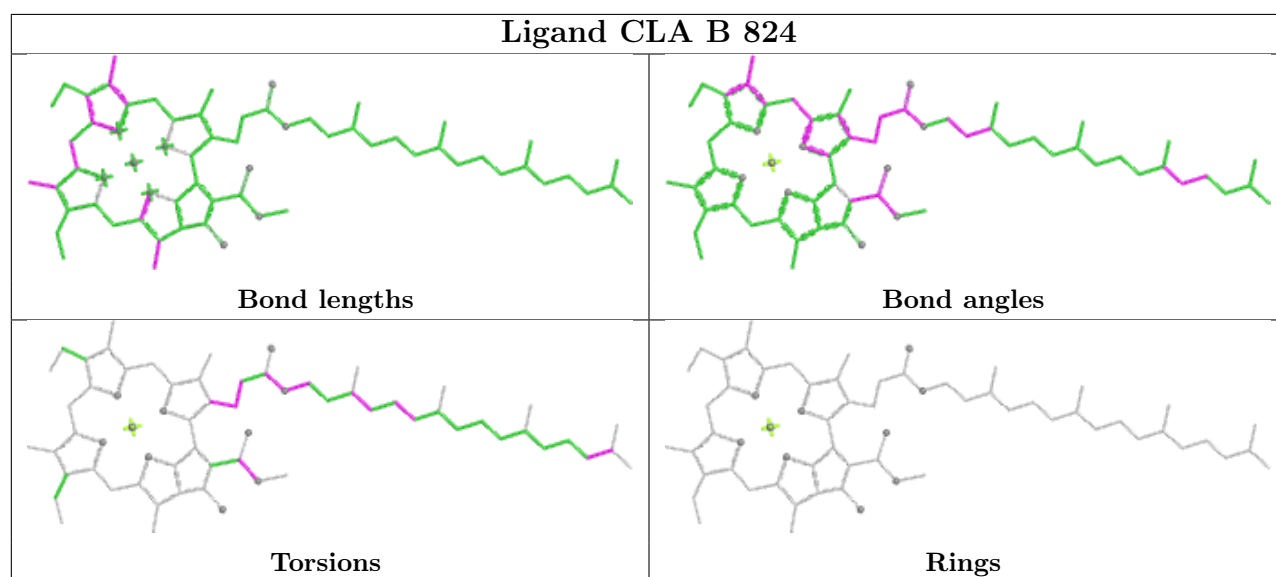
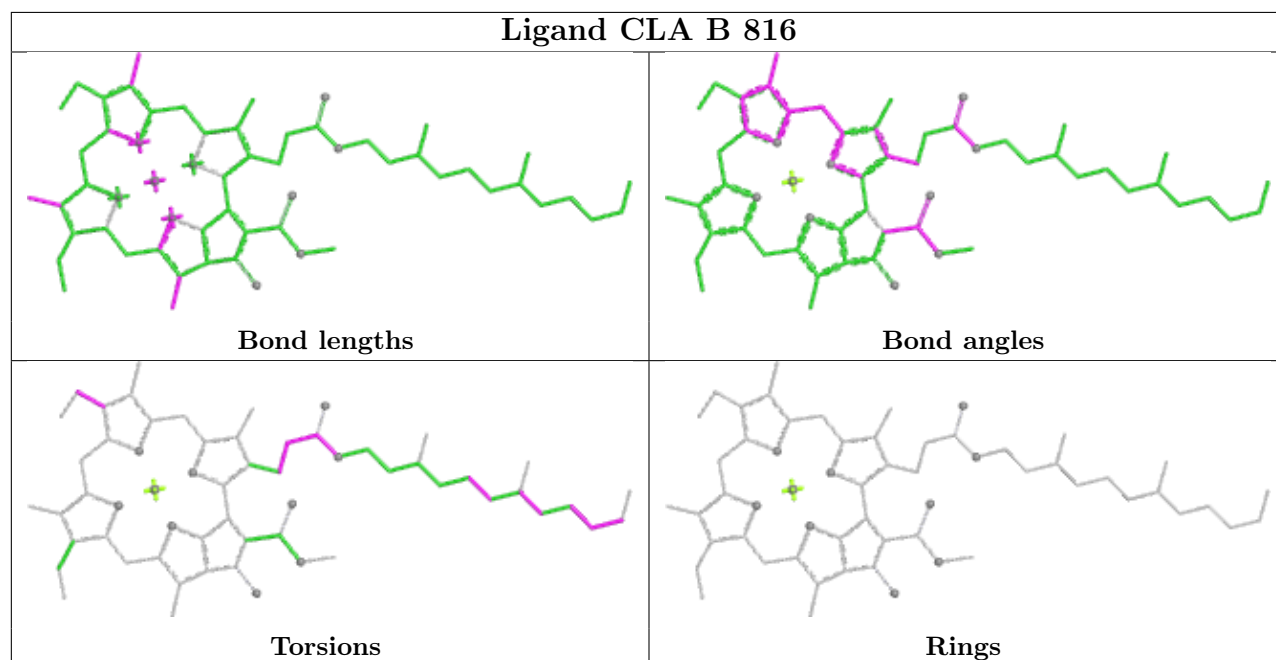
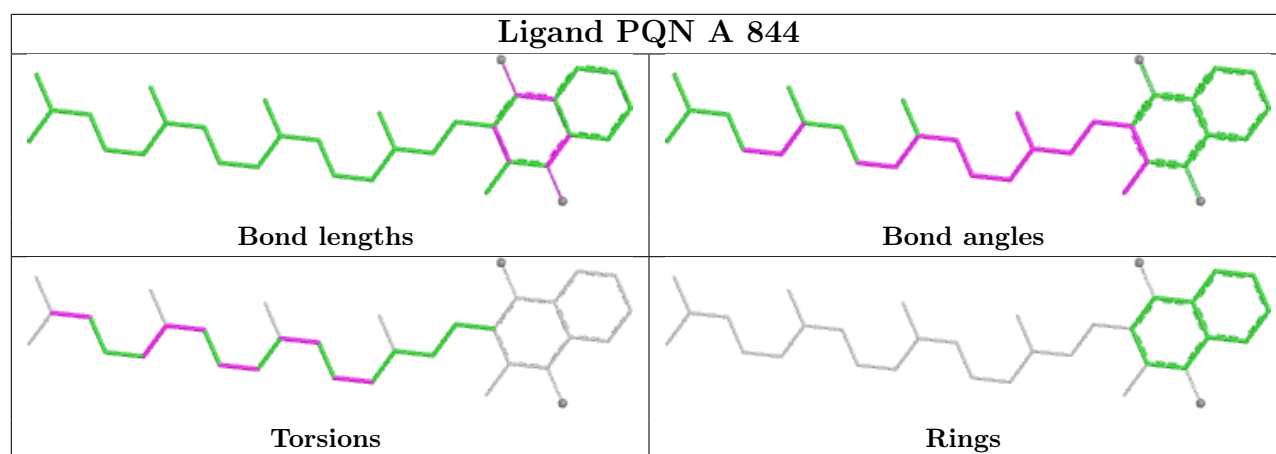


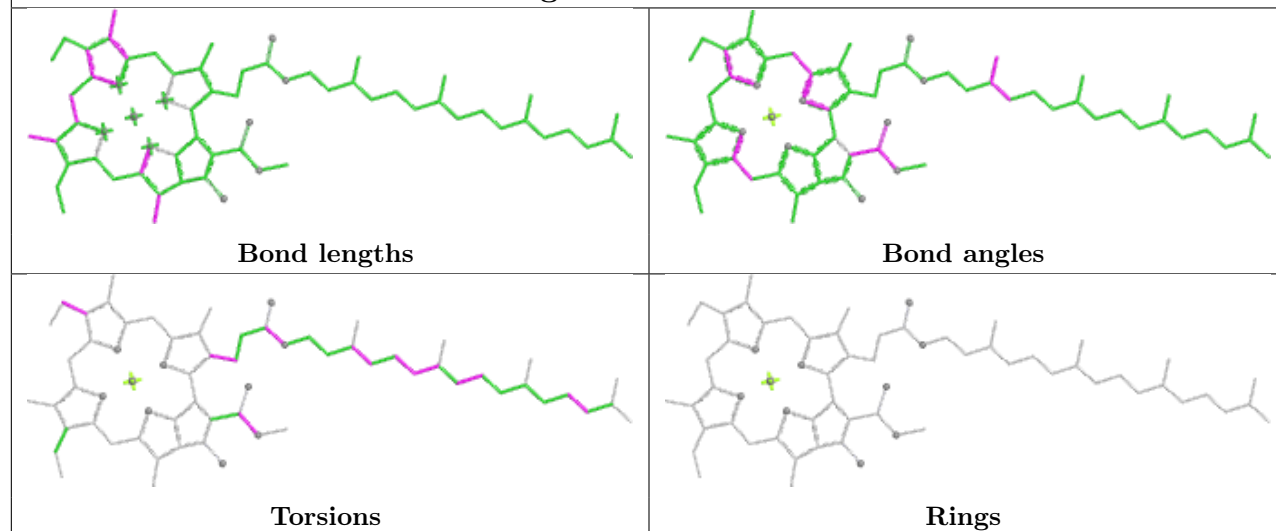
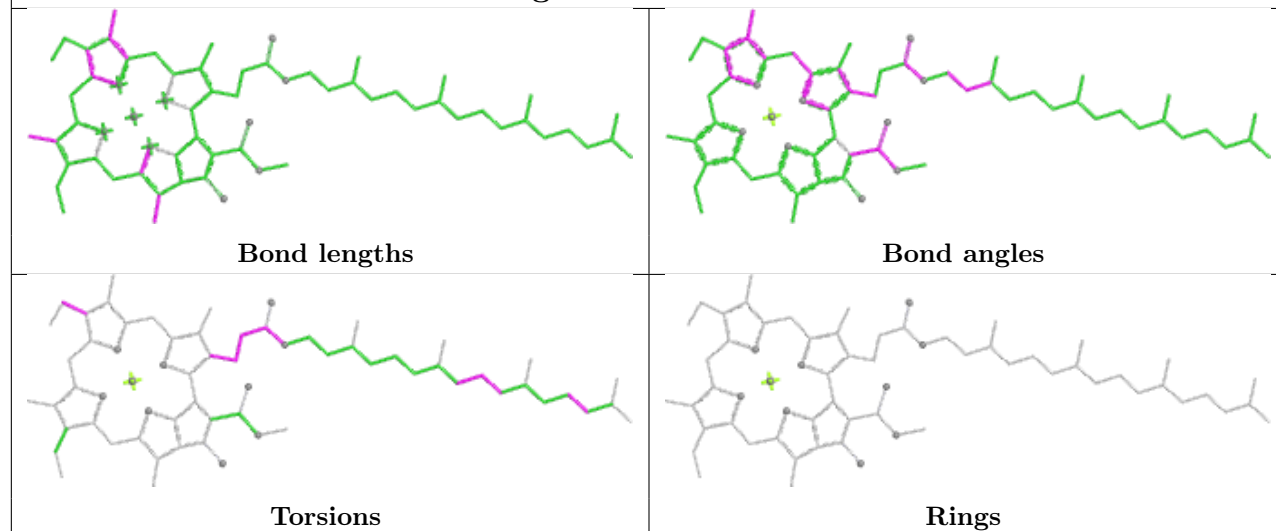
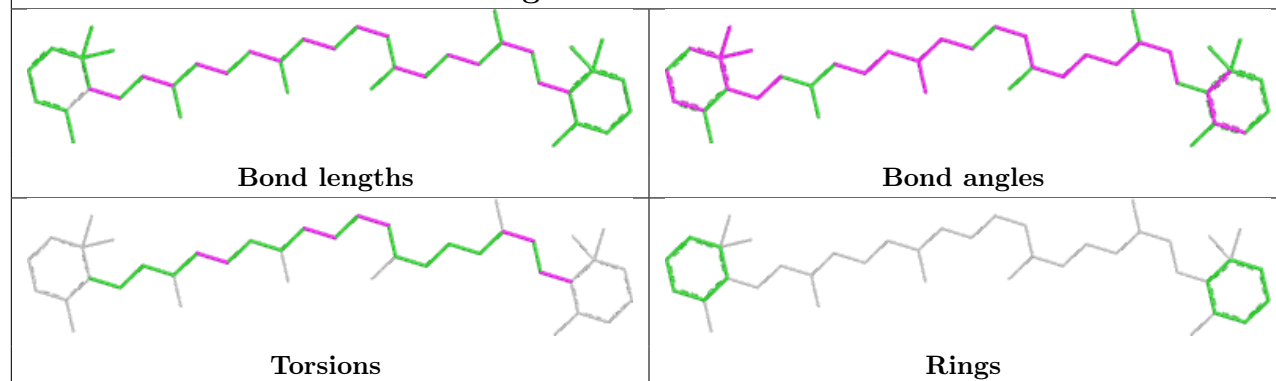


**Ligand CLA a 311****Ligand CLA A 837****Ligand II0 i 313**

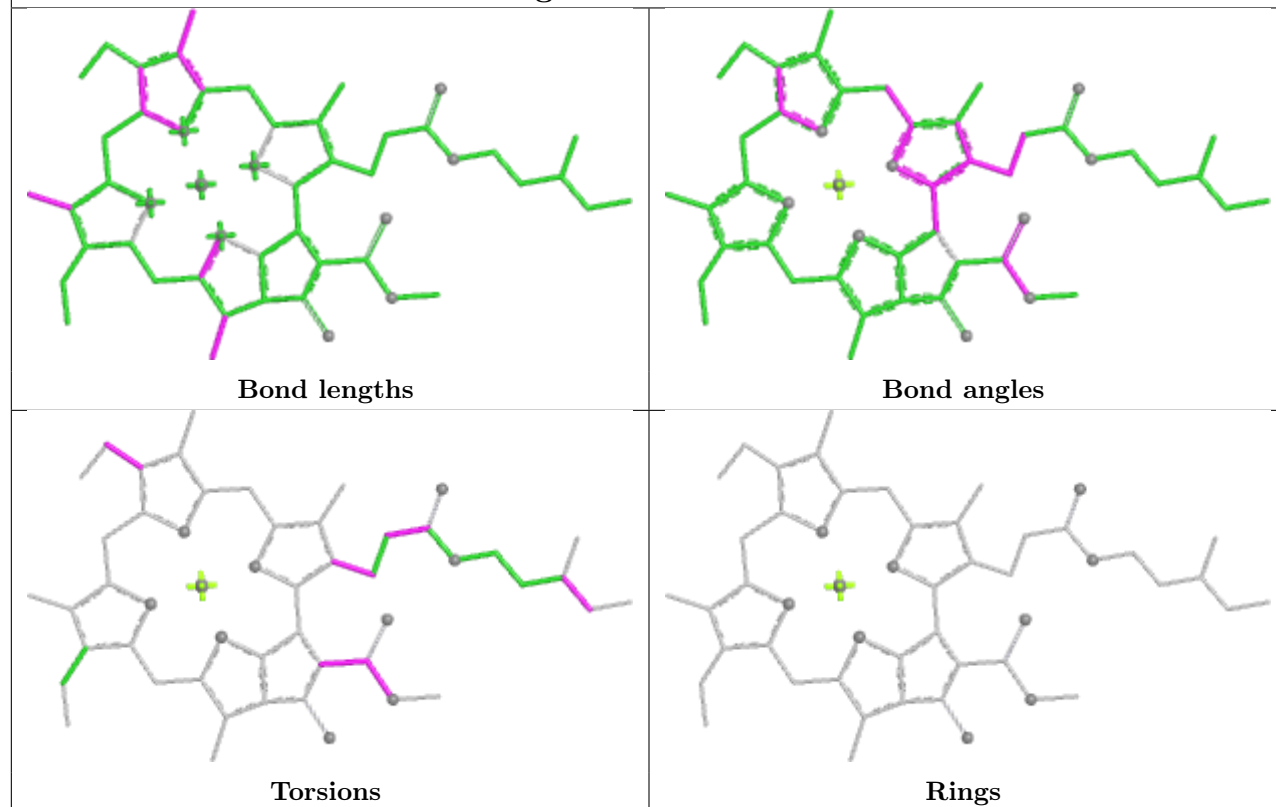




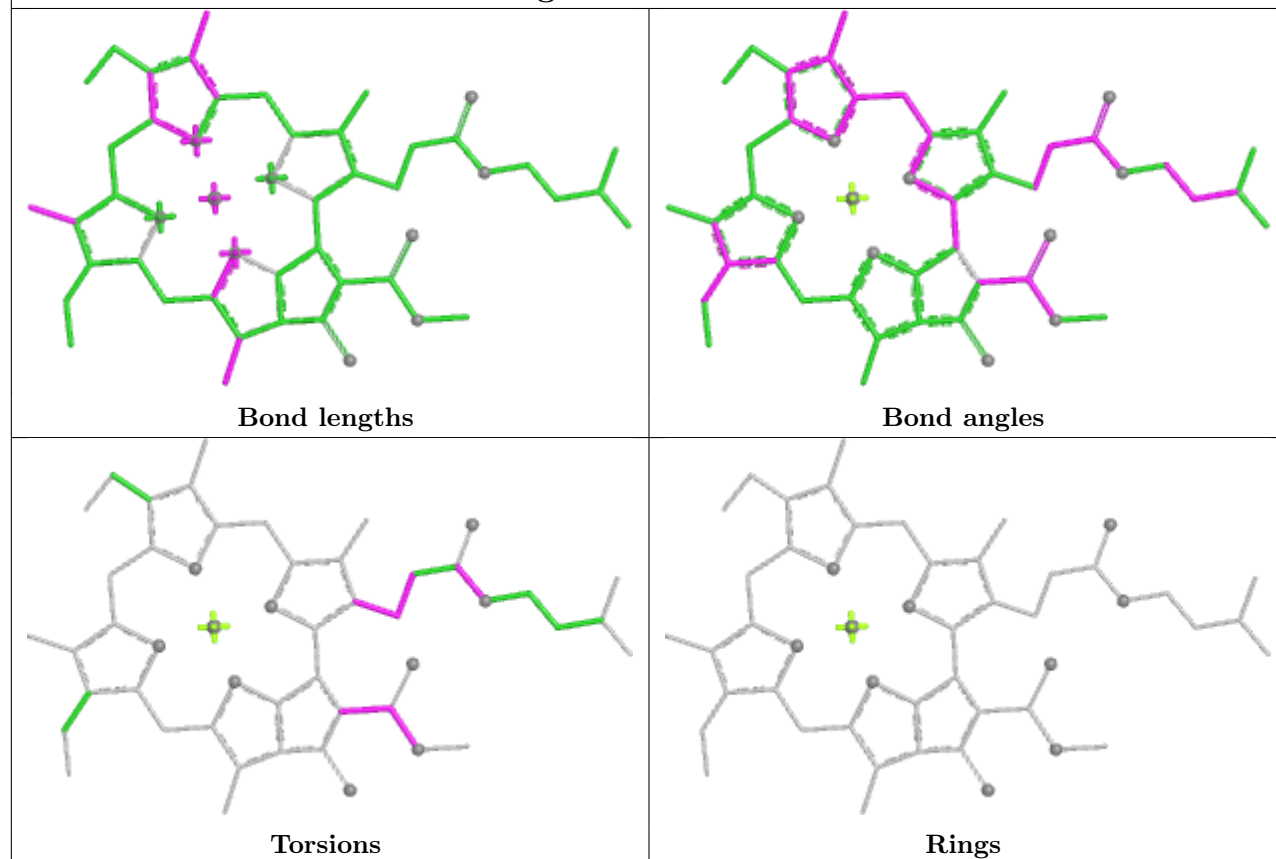


**Ligand CLA I 312****Ligand CLA B 805****Ligand WVN K 103**

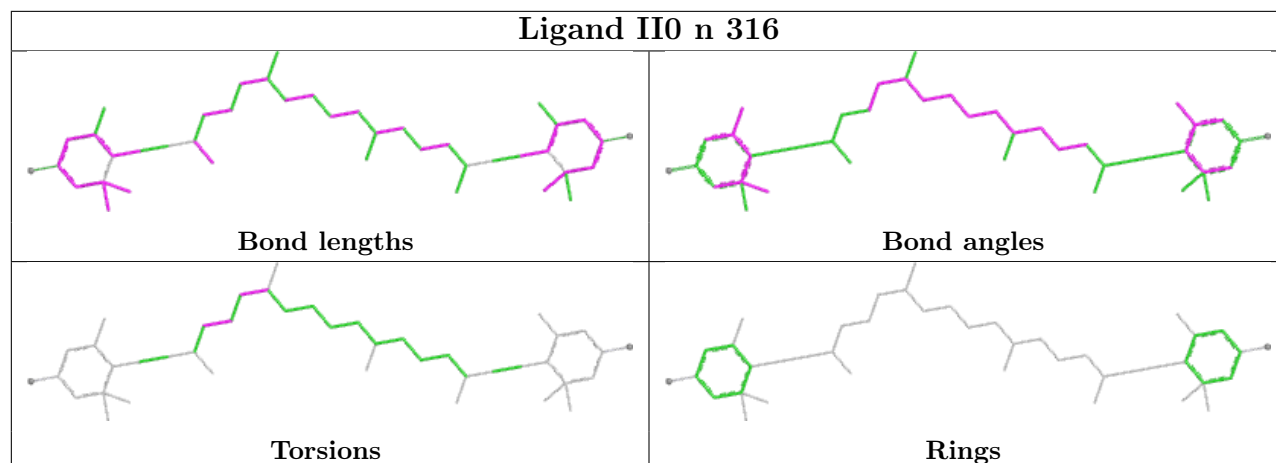
## Ligand CLA h 308



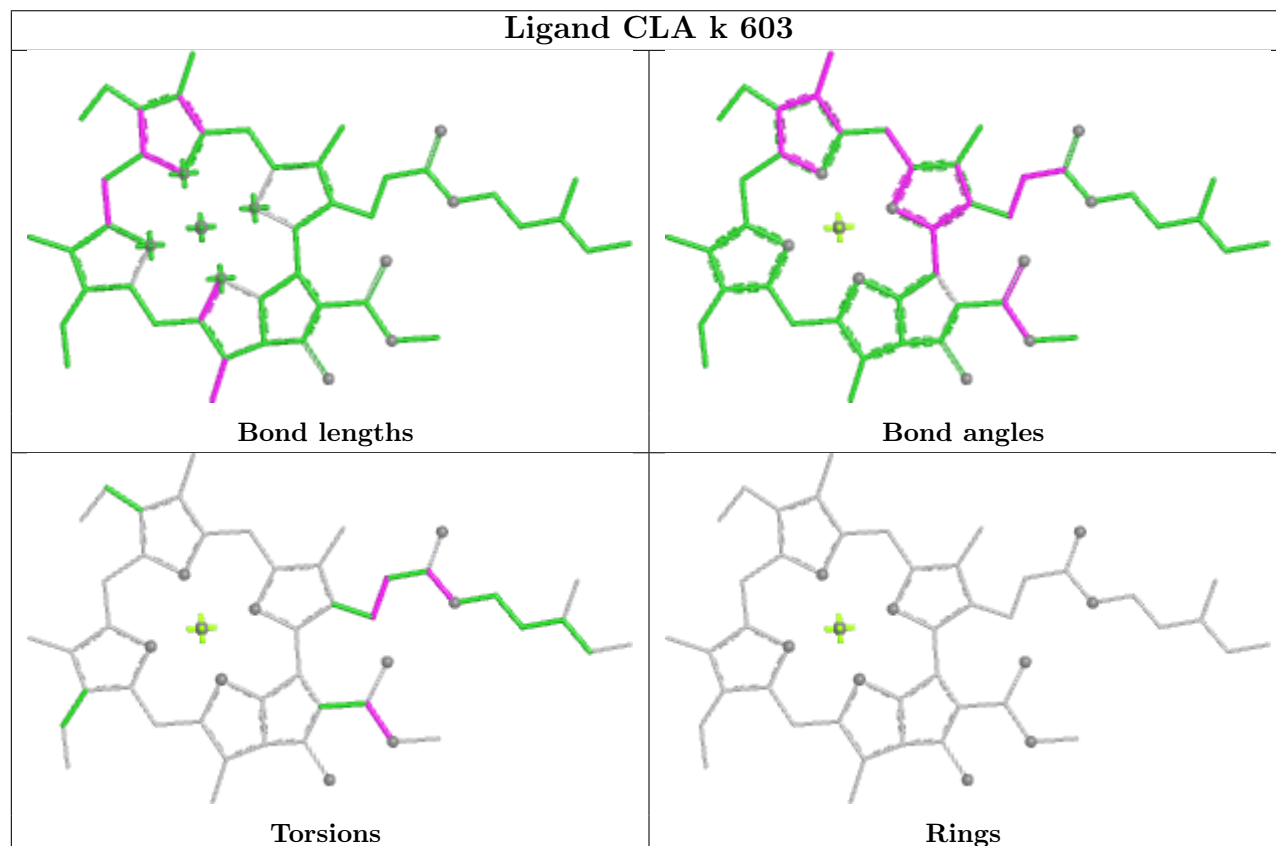
## Ligand CLA c 602



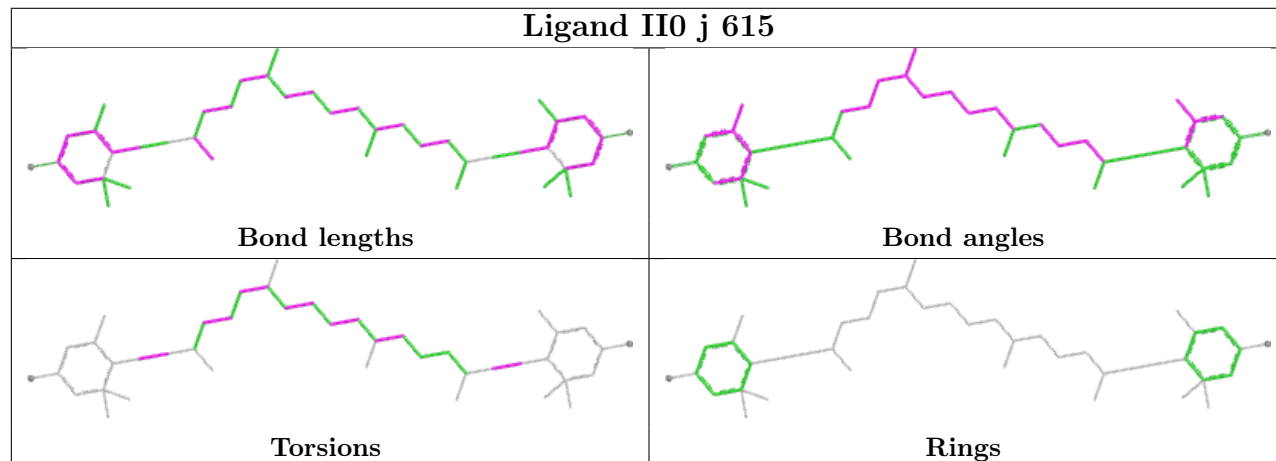
## Ligand II0 n 316

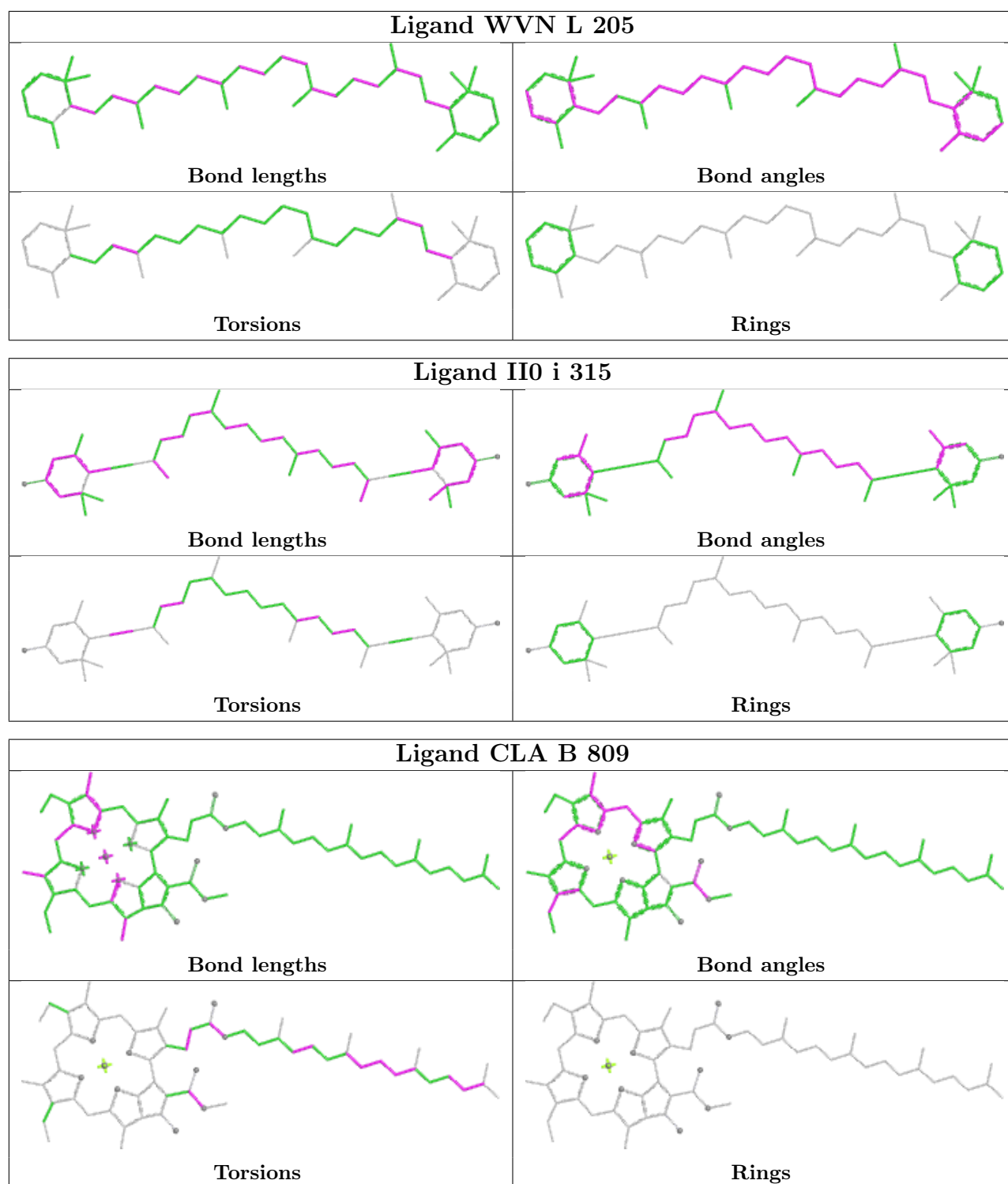


## Ligand CLA k 603

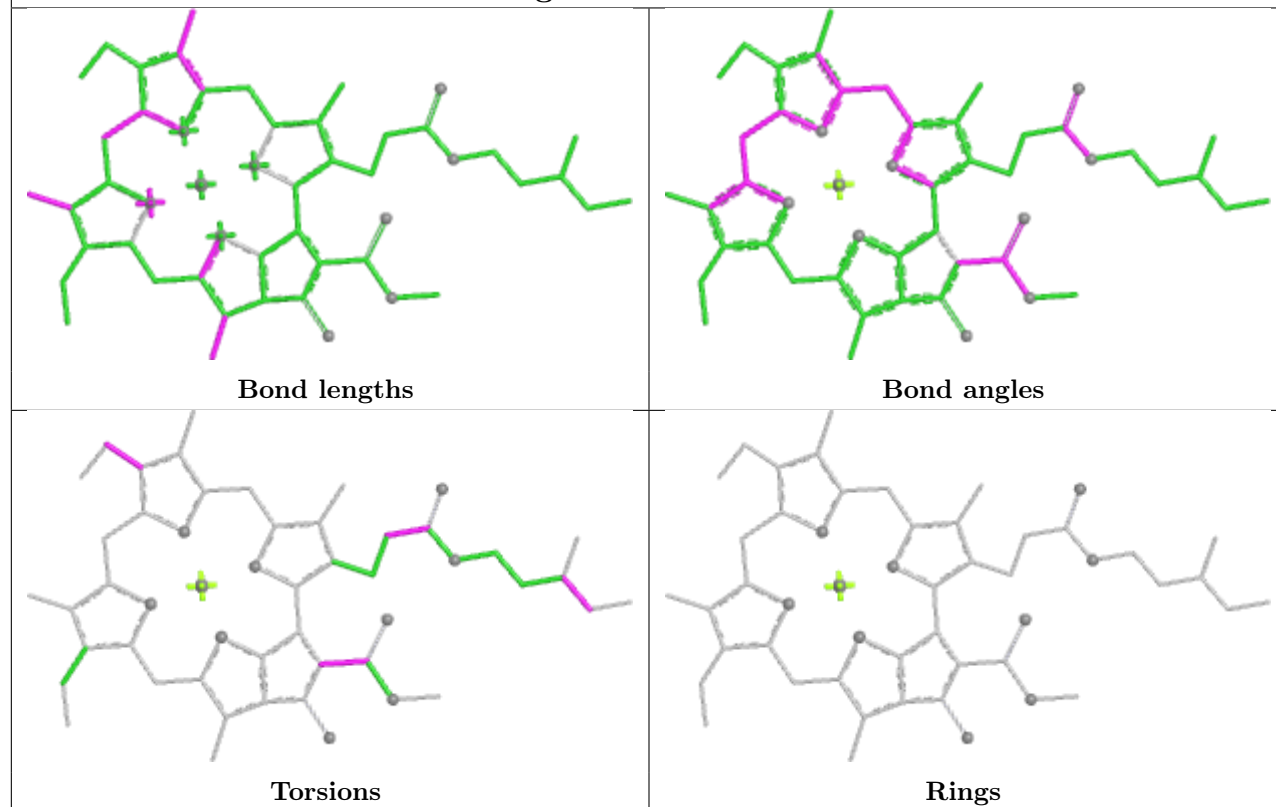


## Ligand II0 j 615

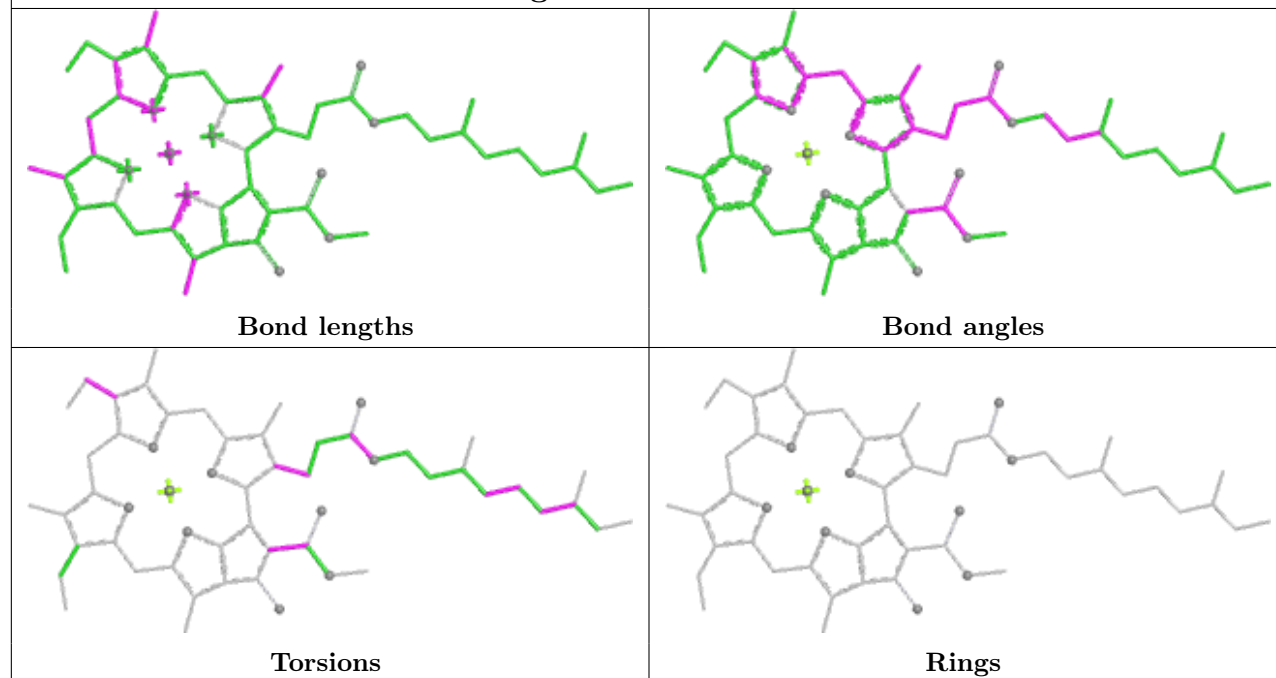




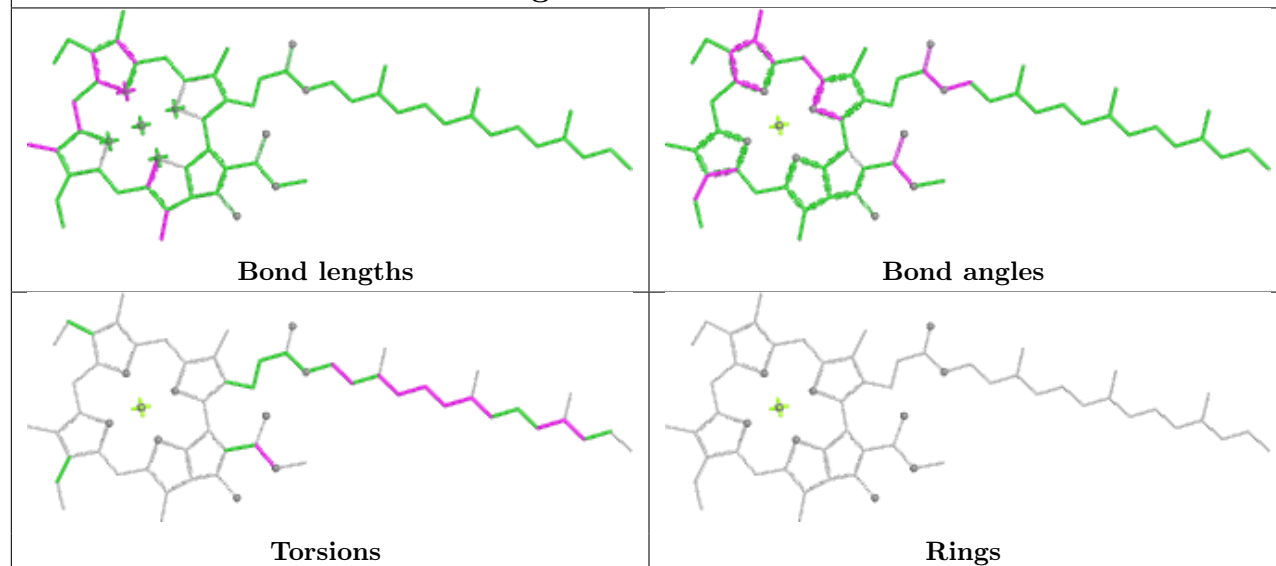
## Ligand CLA d 305



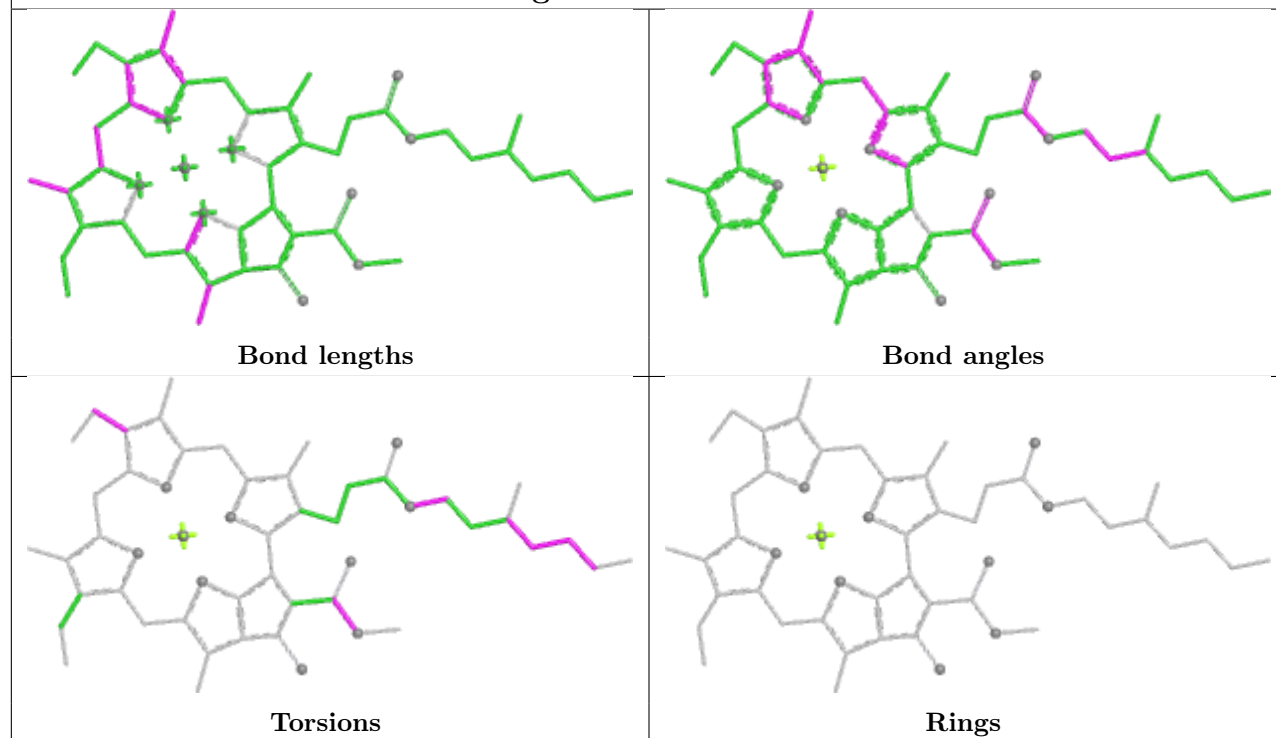
## Ligand CLA m 602



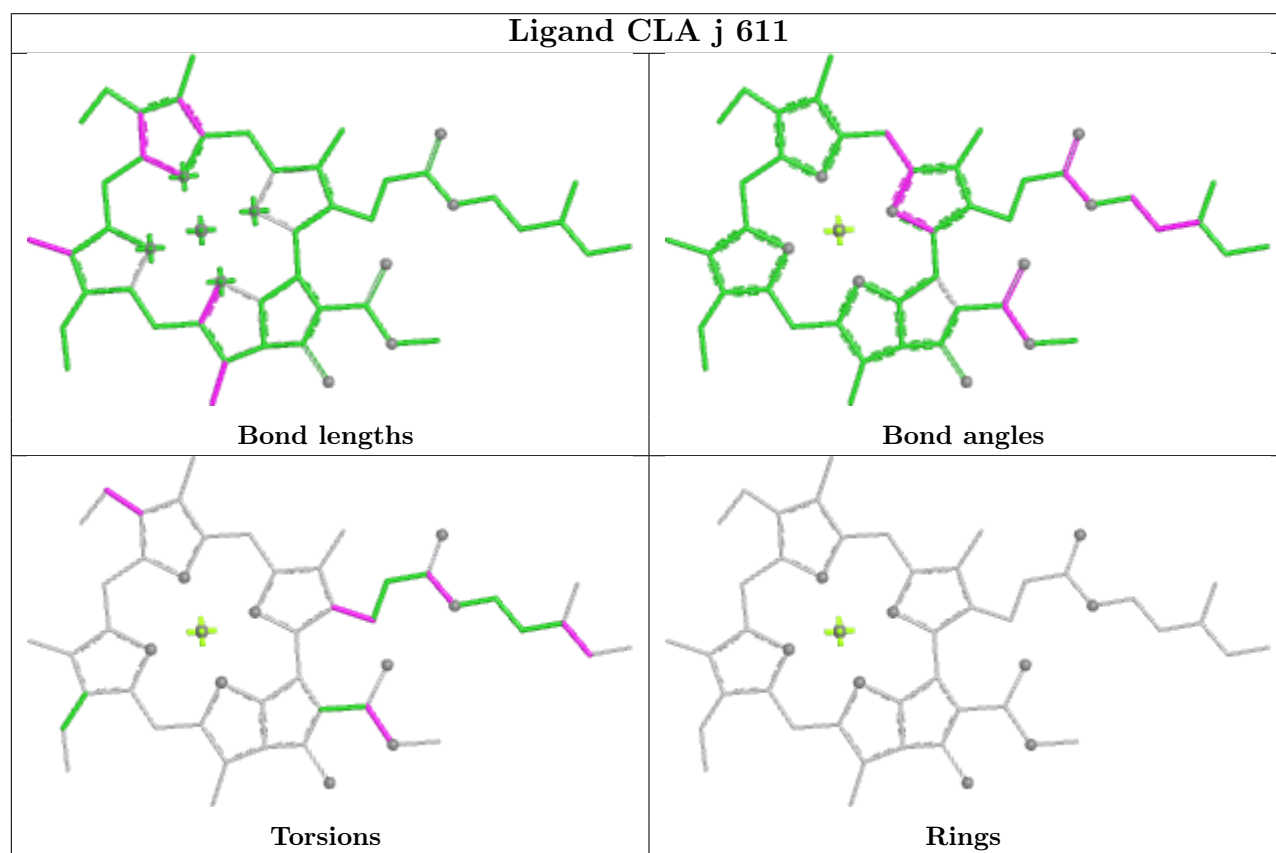
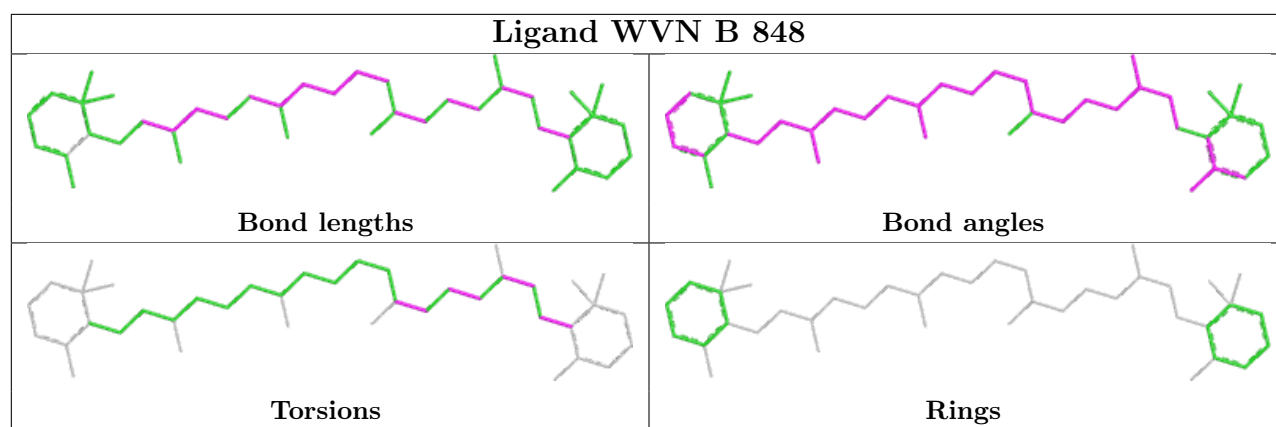
## Ligand CLA A 827



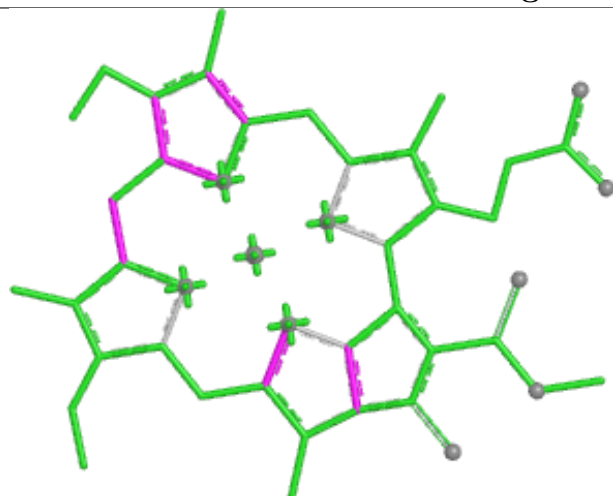
## Ligand CLA B 821



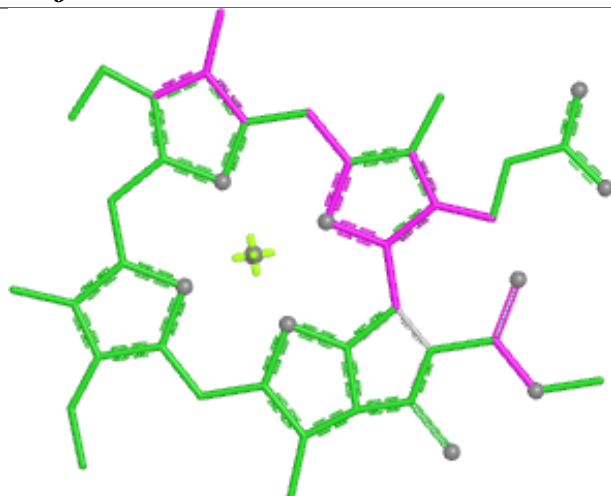




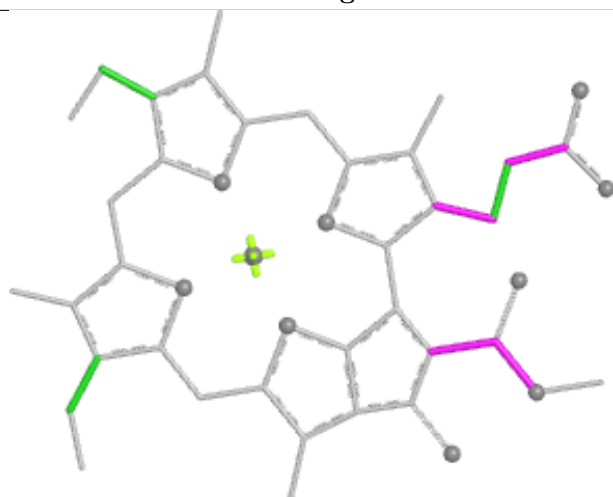
## Ligand CLA j 605



Bond lengths



Bond angles

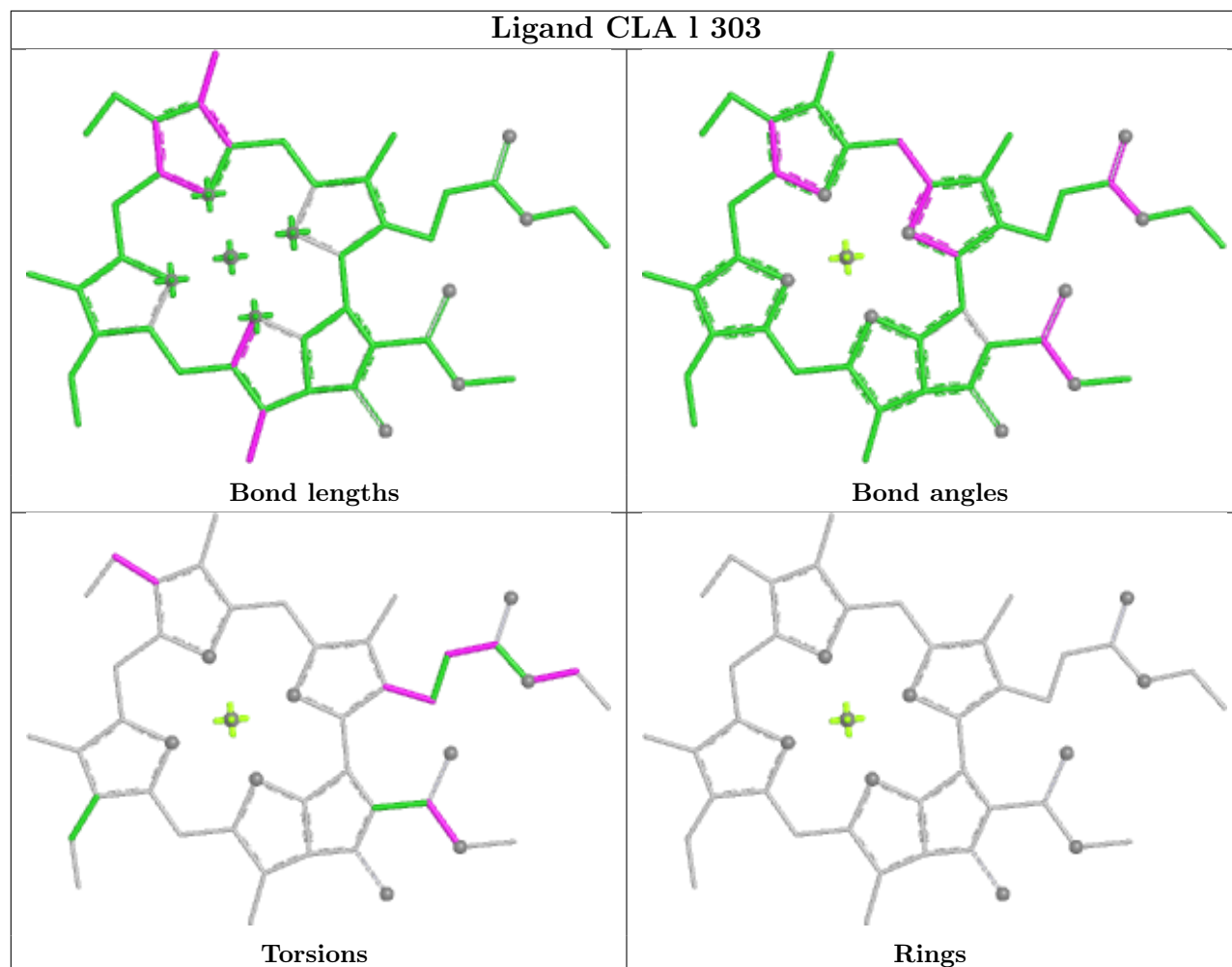


Torsions

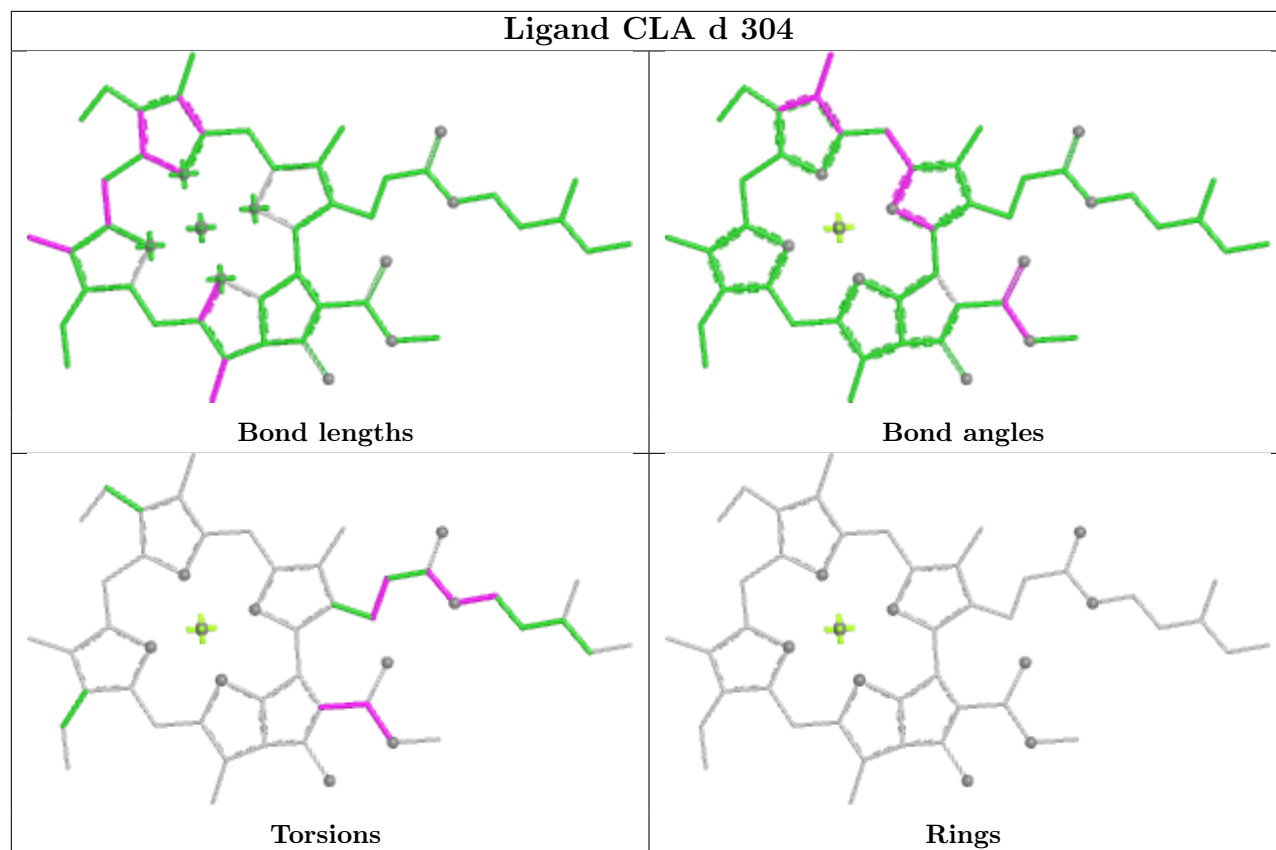


Rings

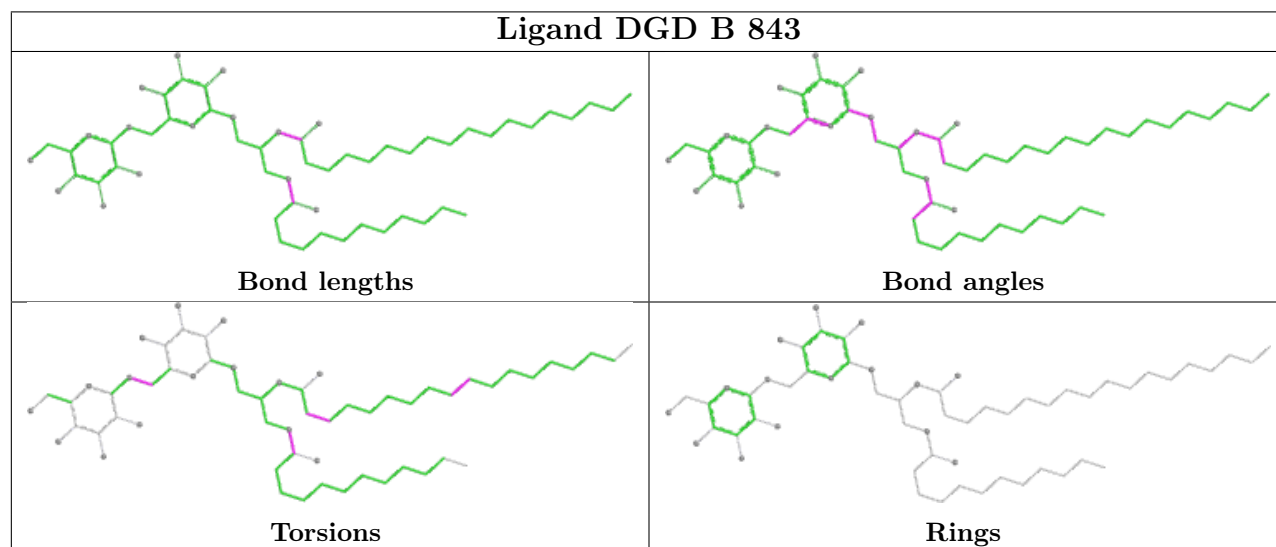
## Ligand CLA 1 303



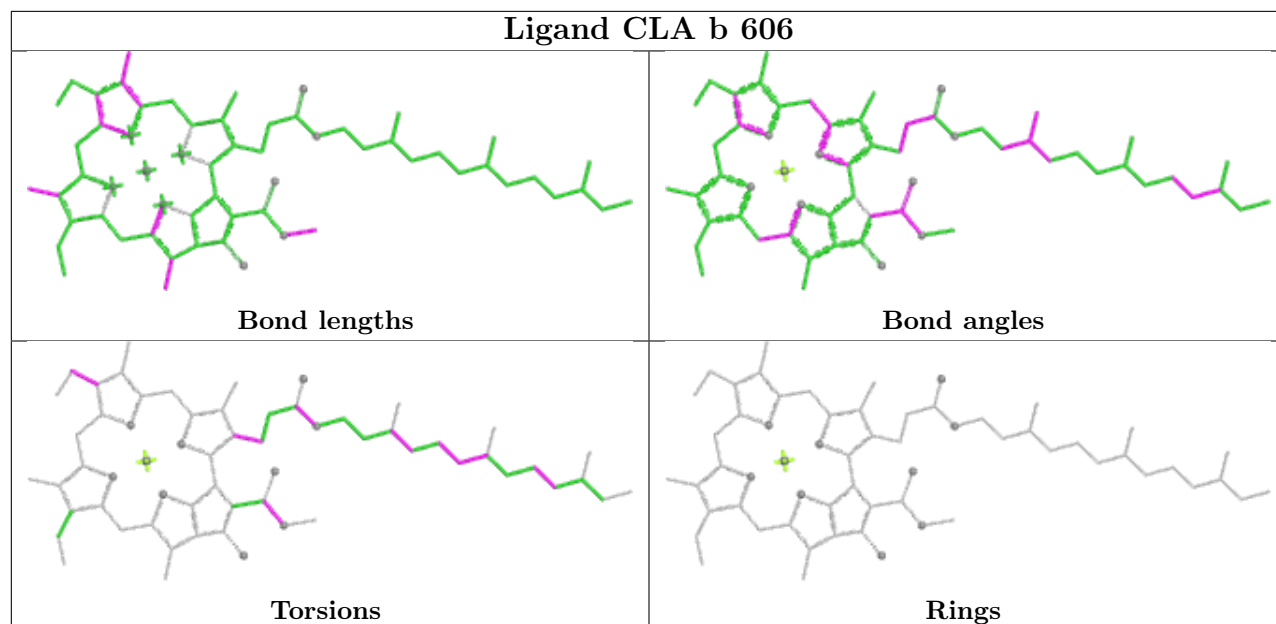
## Ligand CLA d 304



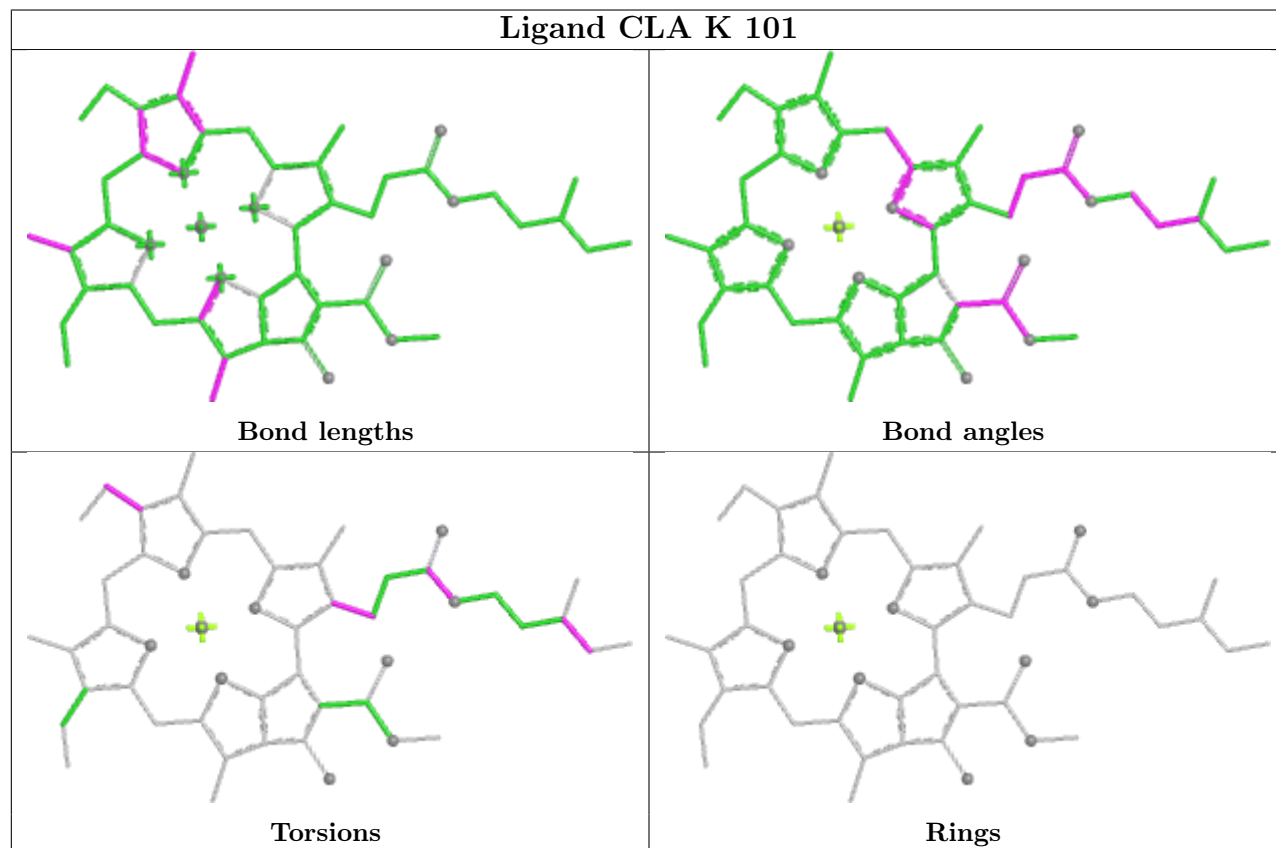
## Ligand DGD B 843

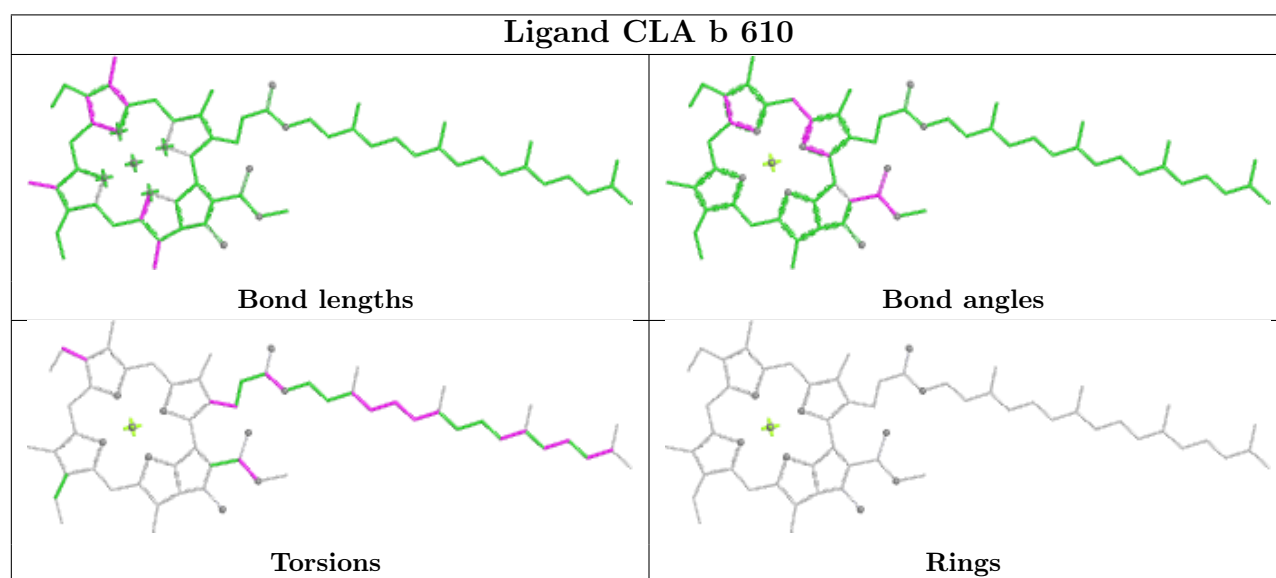
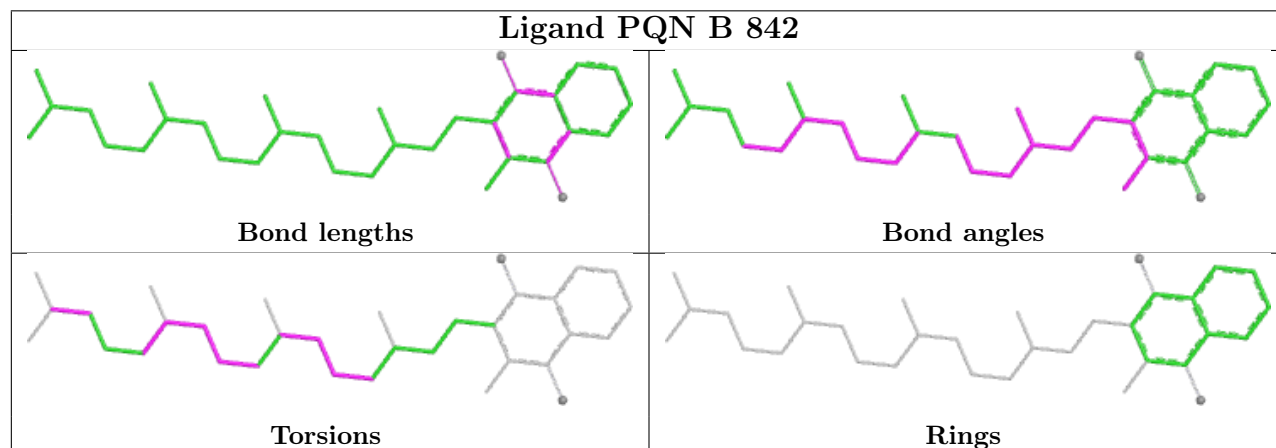
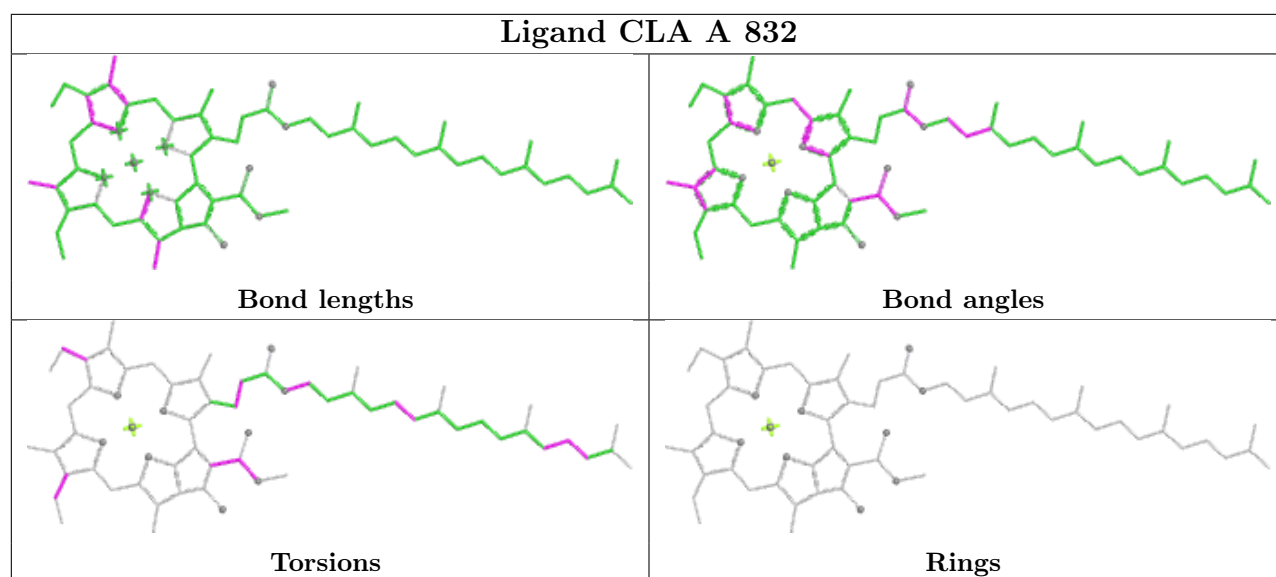


## Ligand CLA b 606

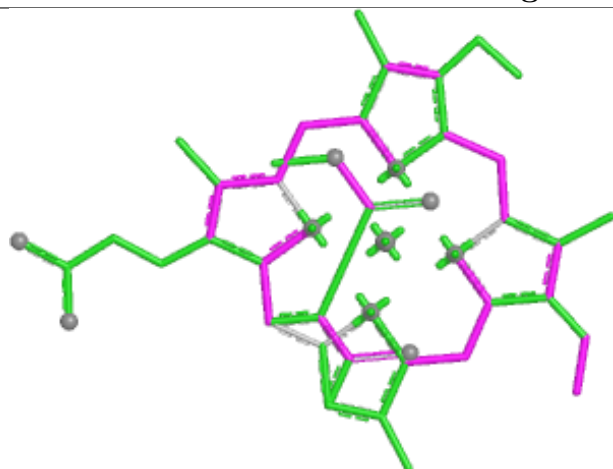


## Ligand CLA K 101

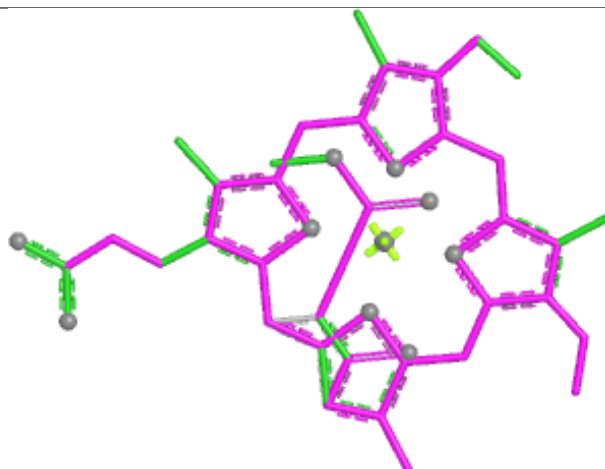




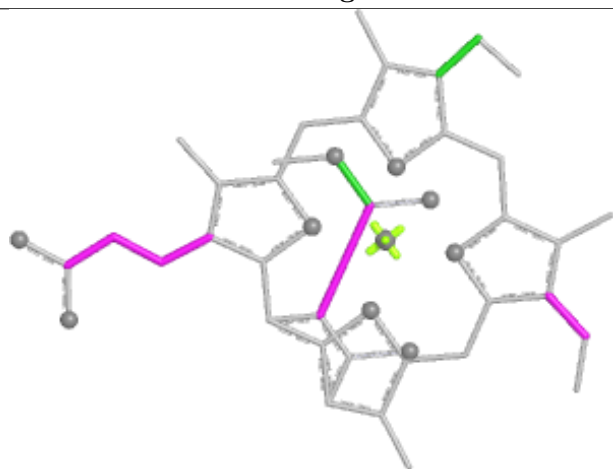
## Ligand KC2 c 610



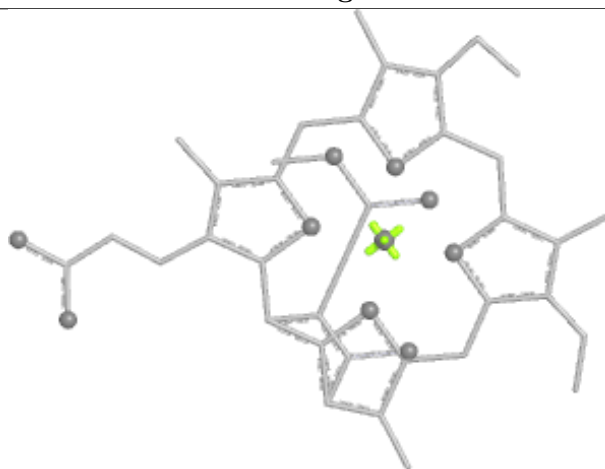
Bond lengths



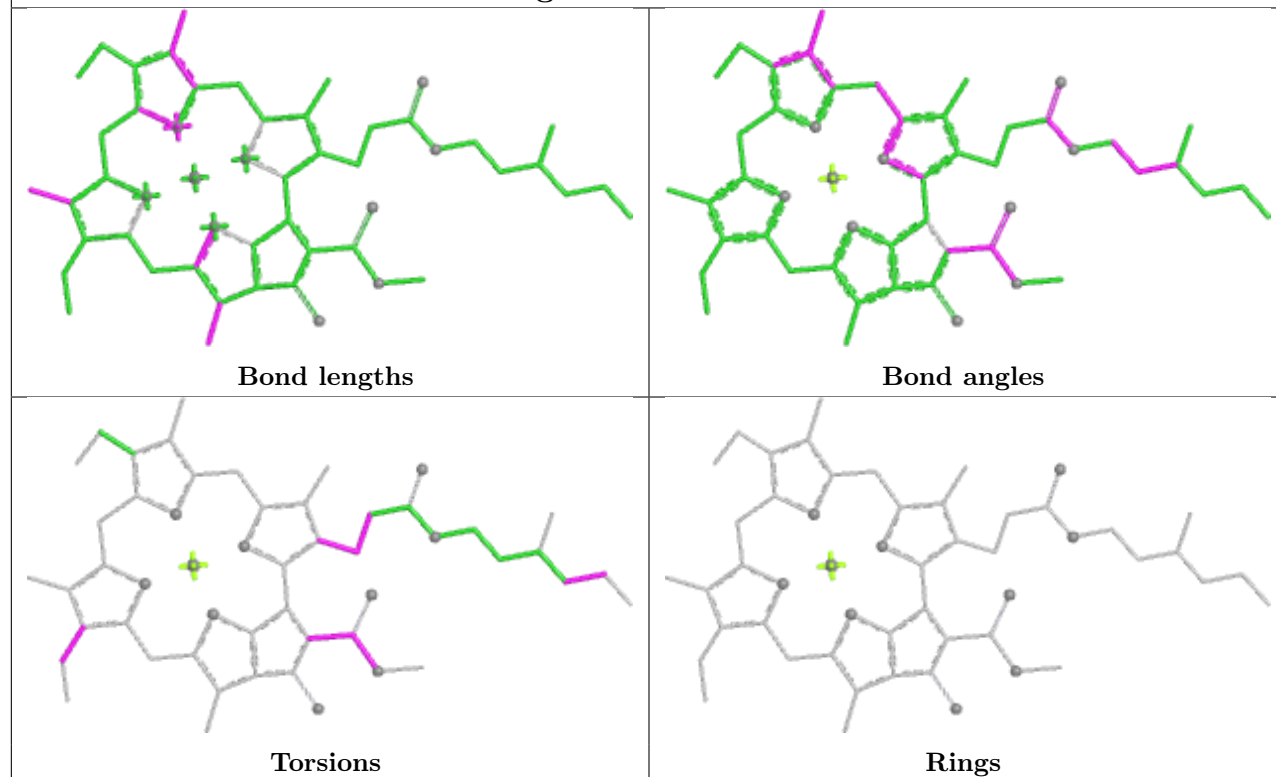
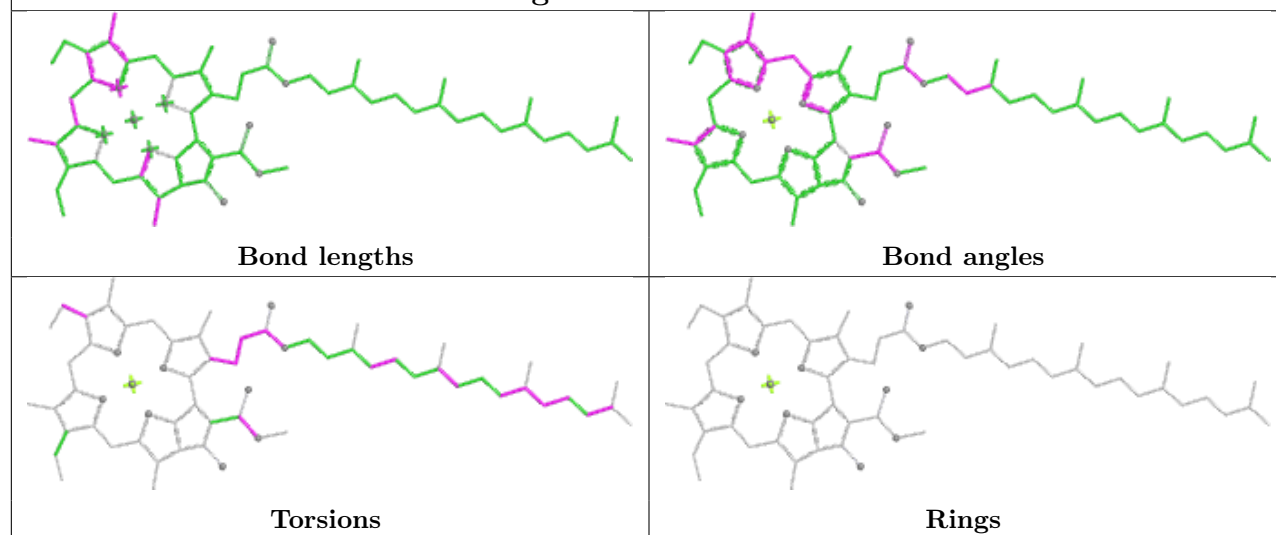
Bond angles



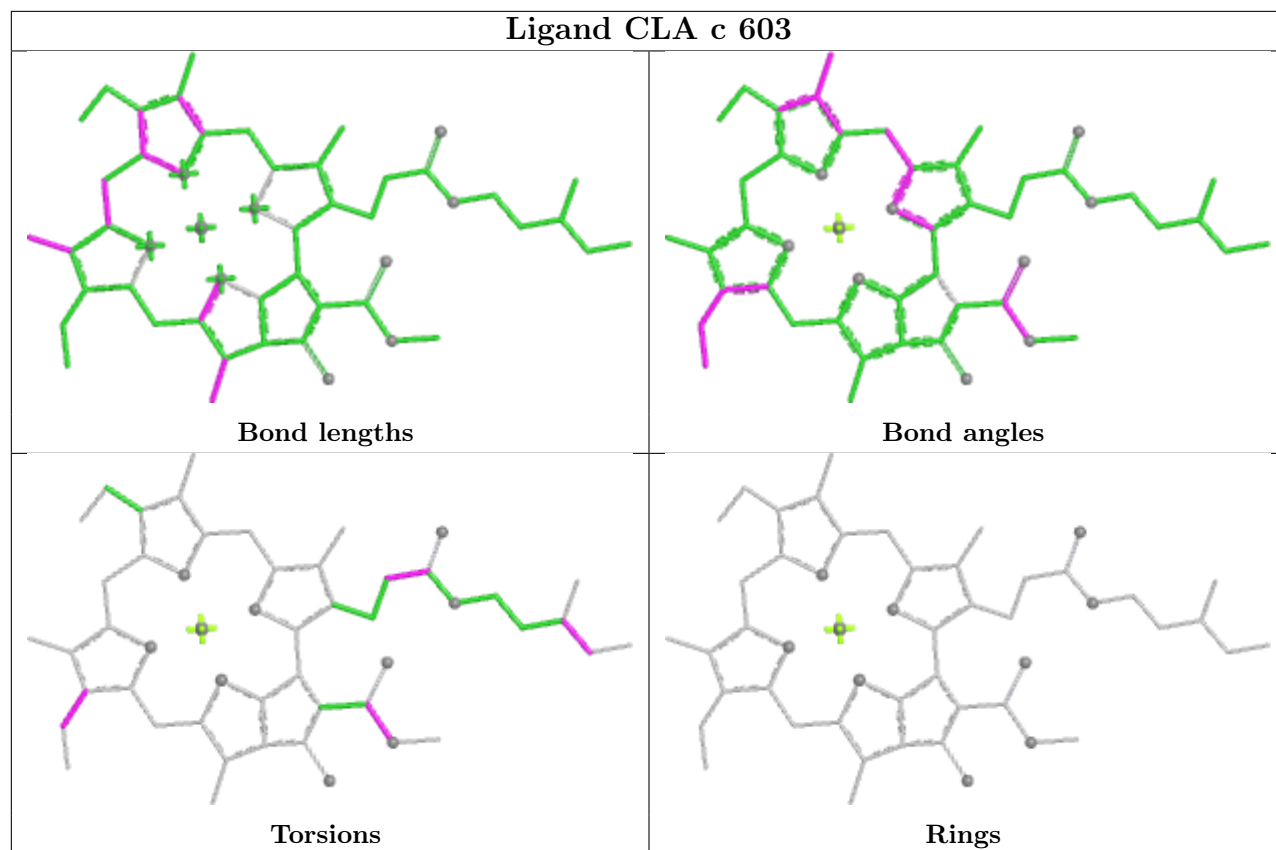
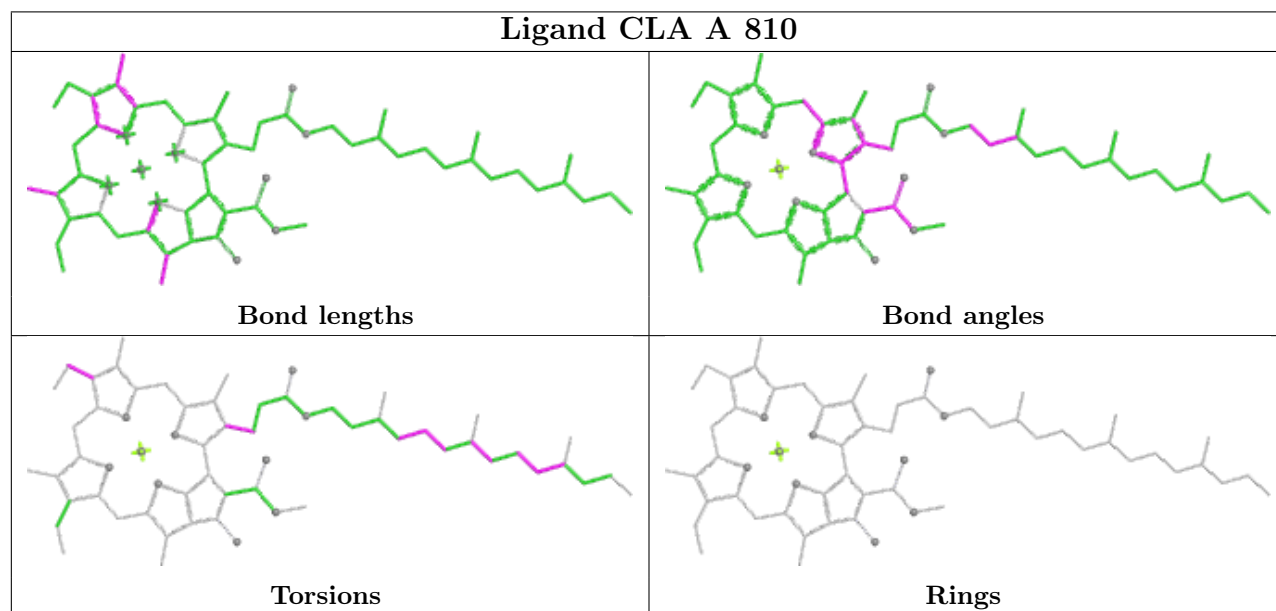
Torsions



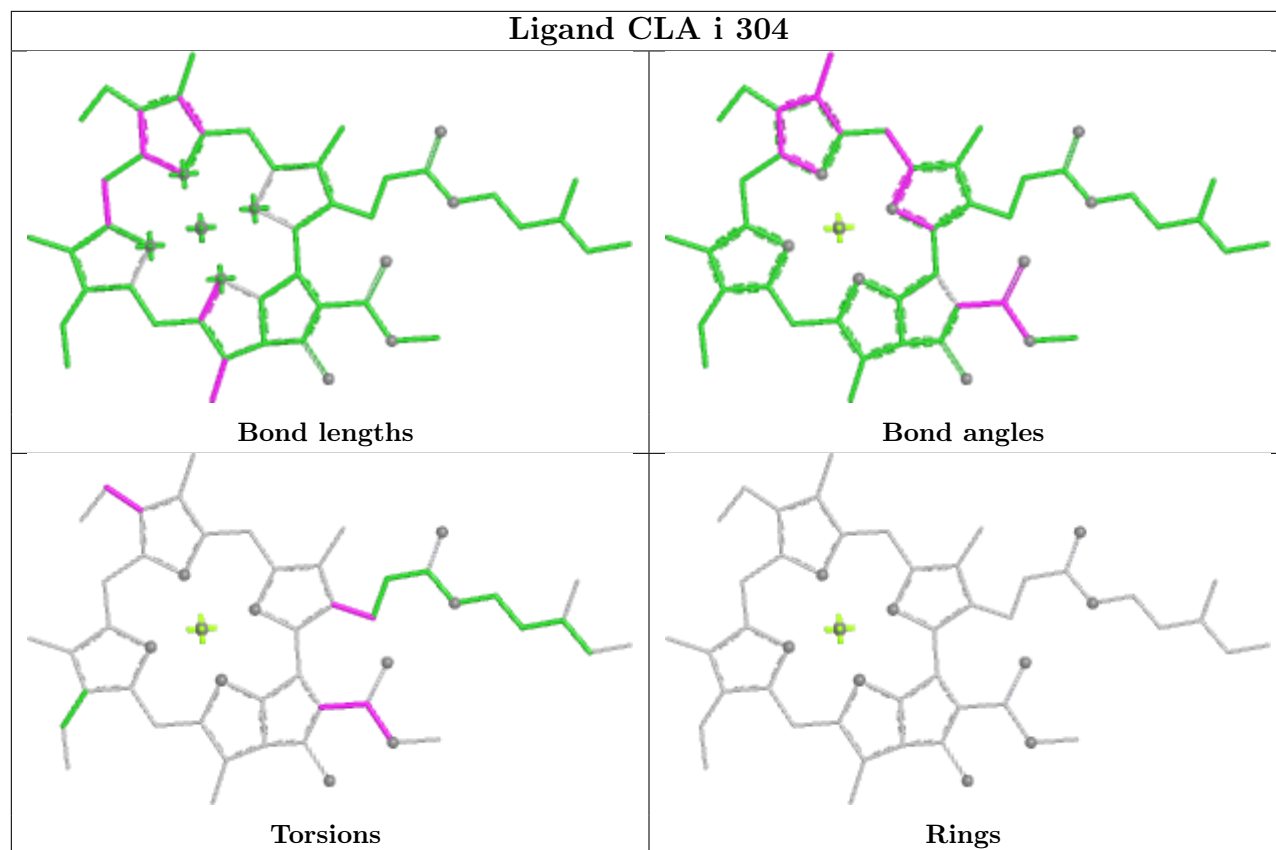
Rings

**Ligand CLA a 303****Ligand CLA A 817**

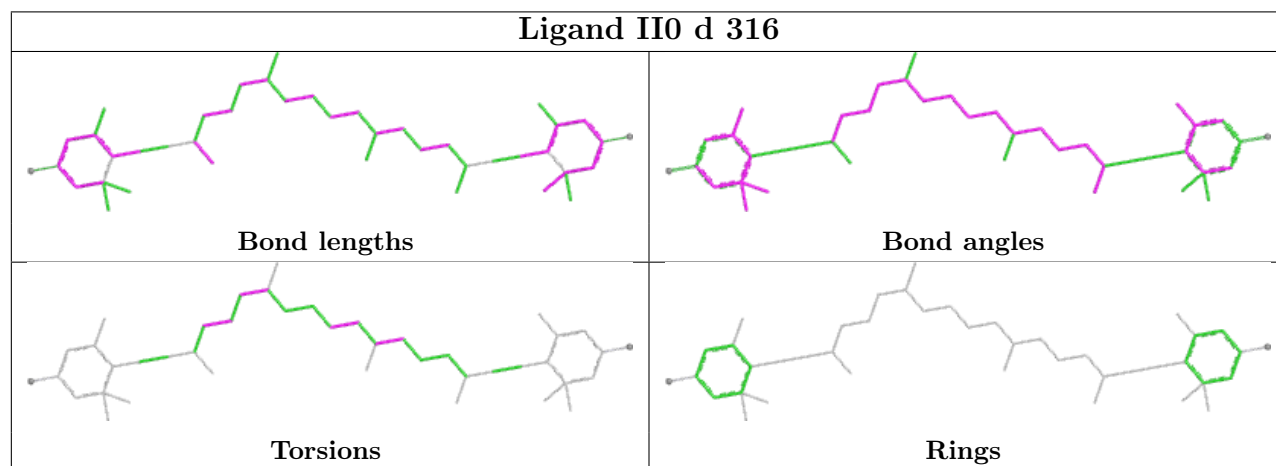


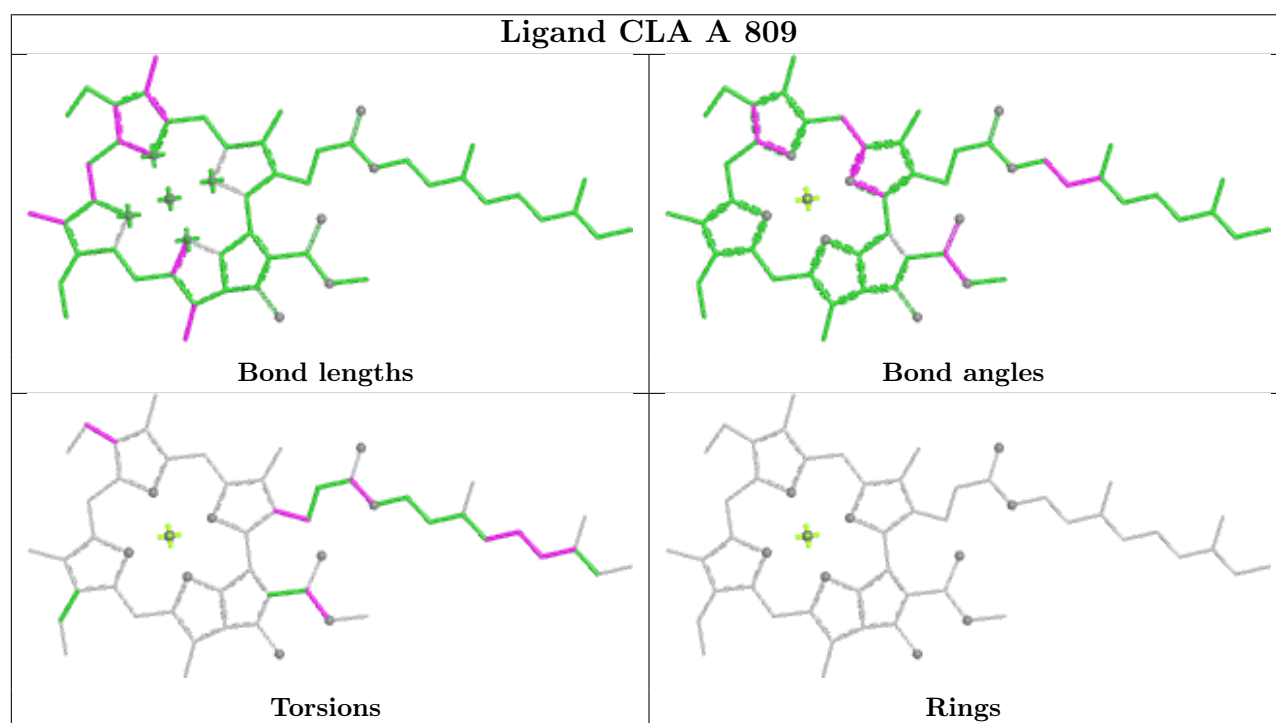
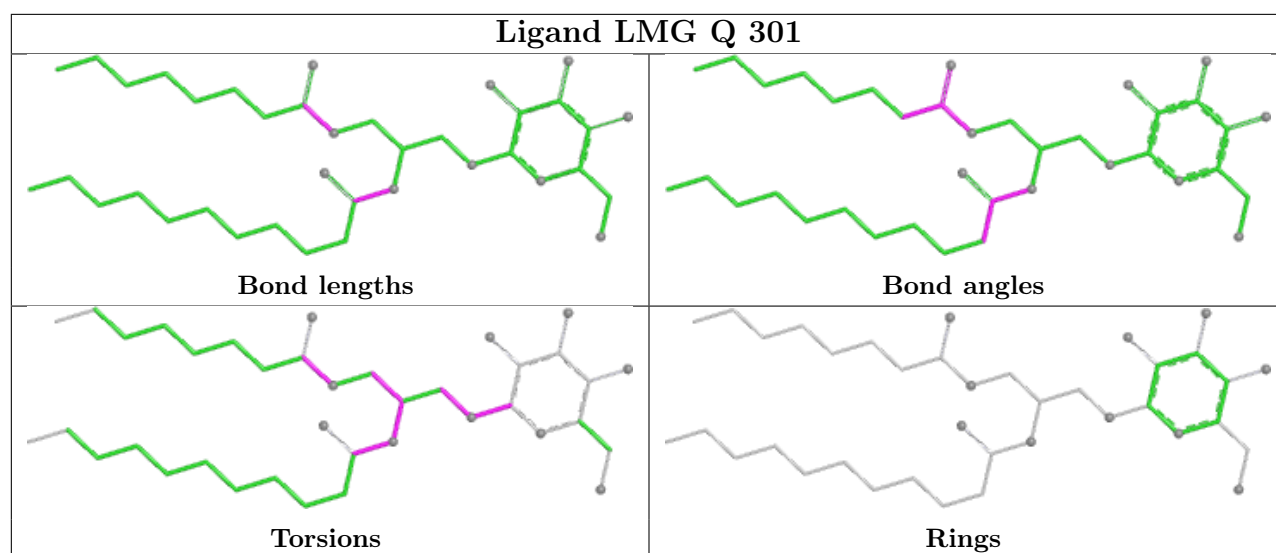
**Ligand CLA c 603****Ligand CLA A 810**

## Ligand CLA i 304

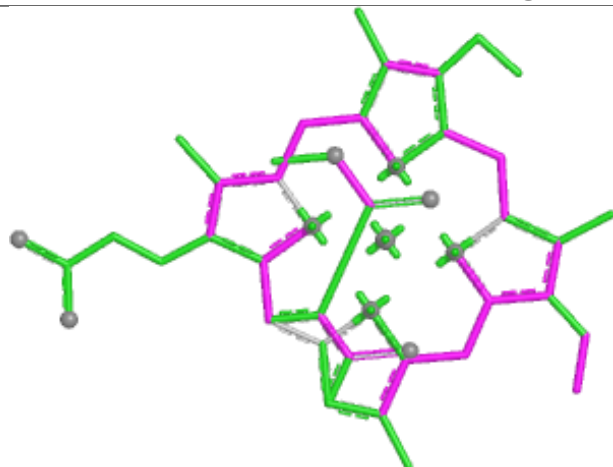


## Ligand II0 d 316

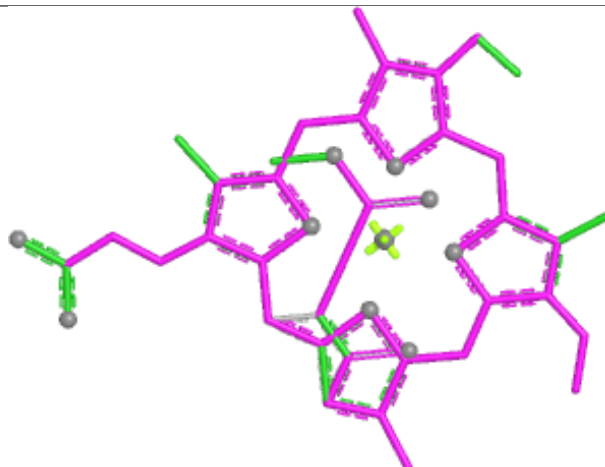




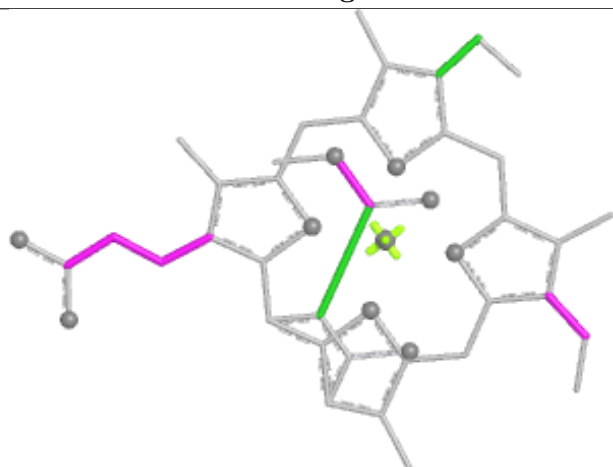
## Ligand KC2 k 611



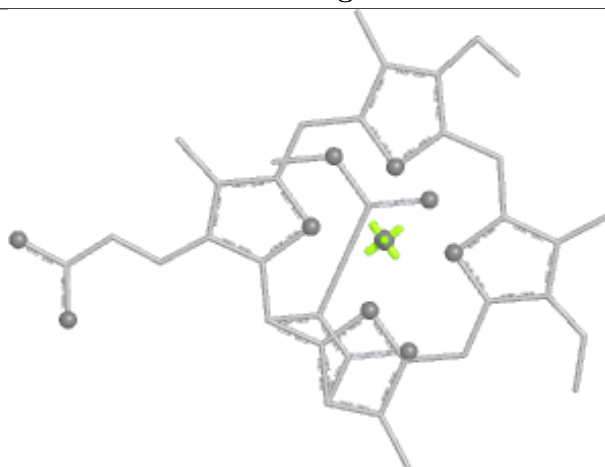
Bond lengths



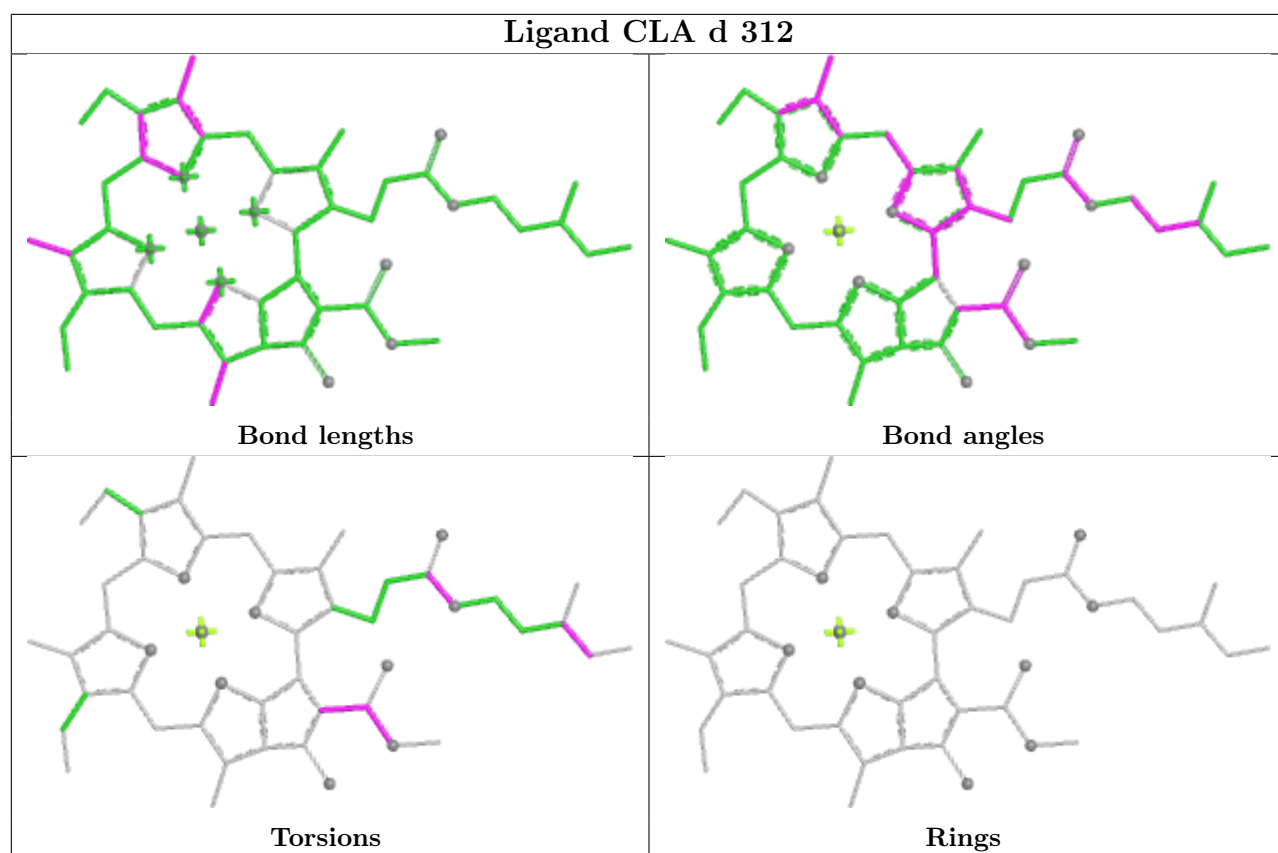
Bond angles

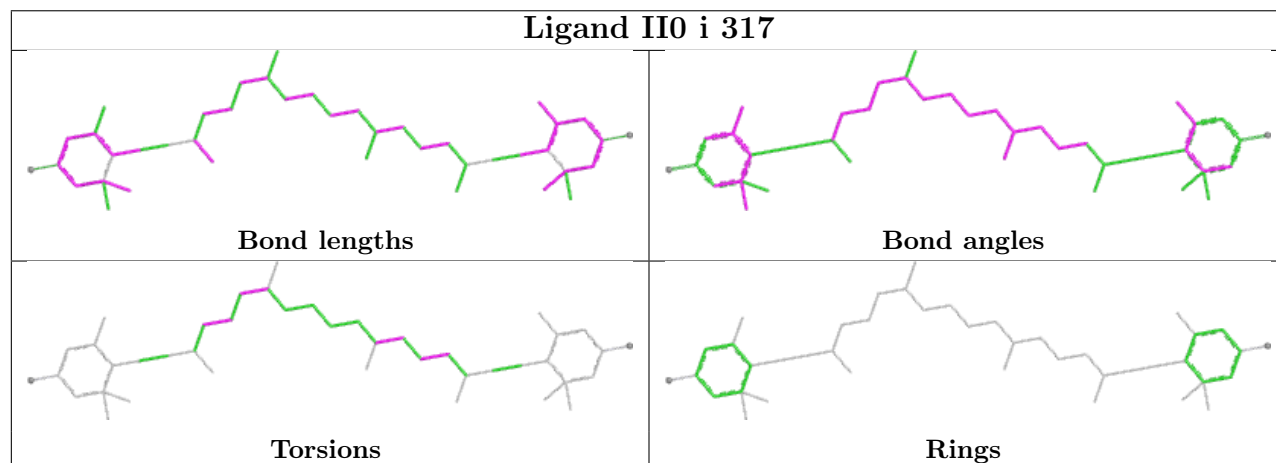
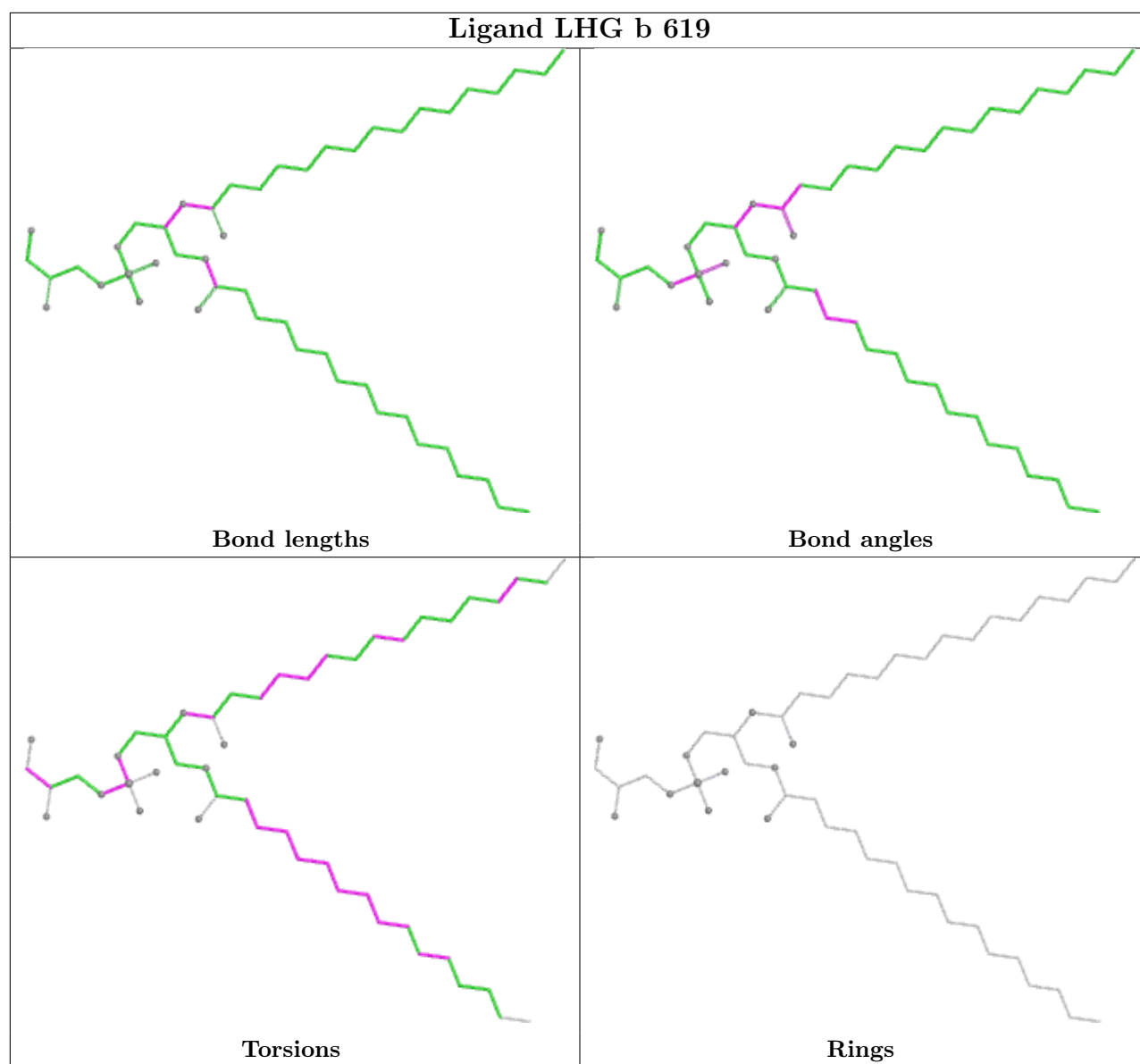


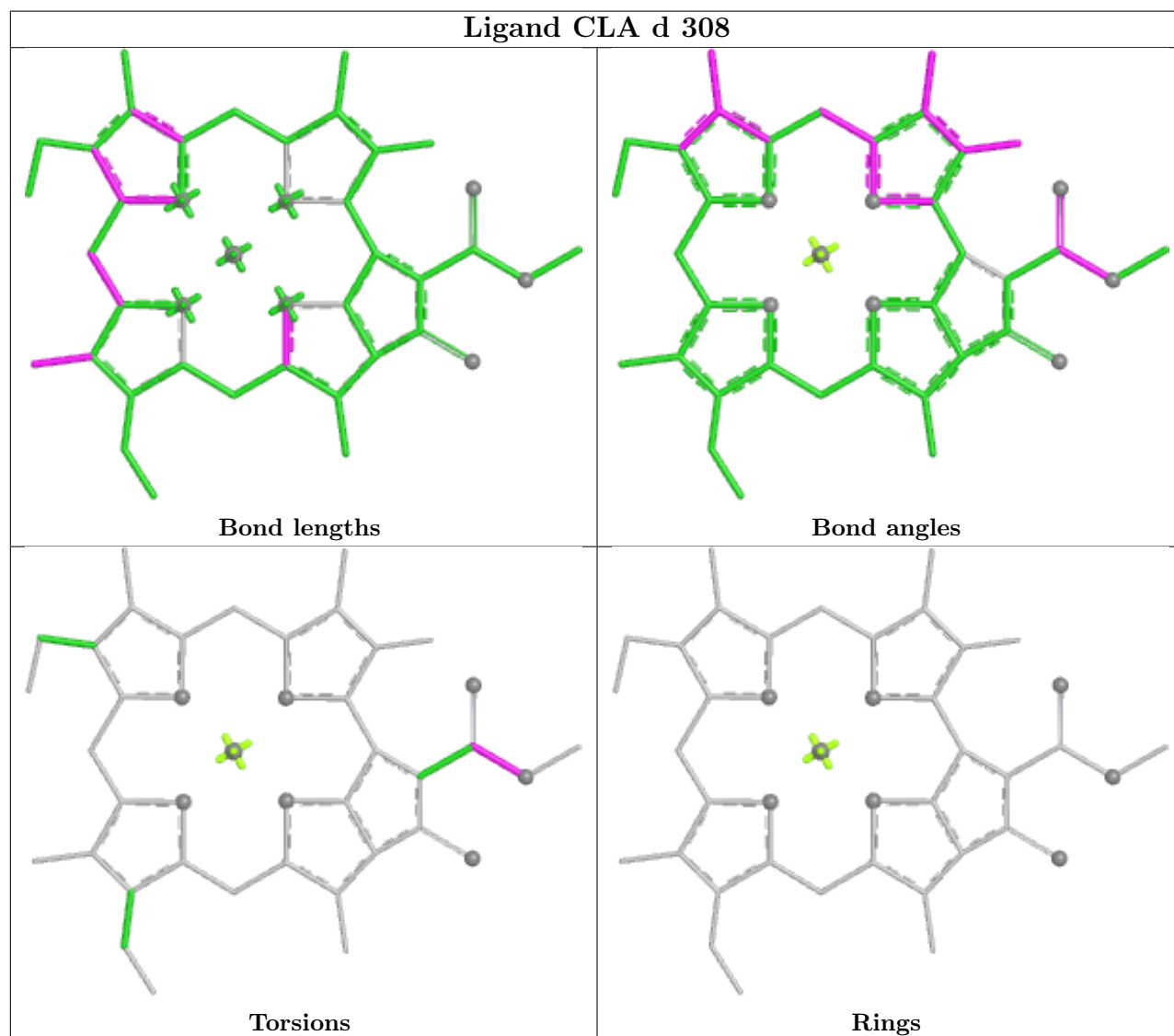
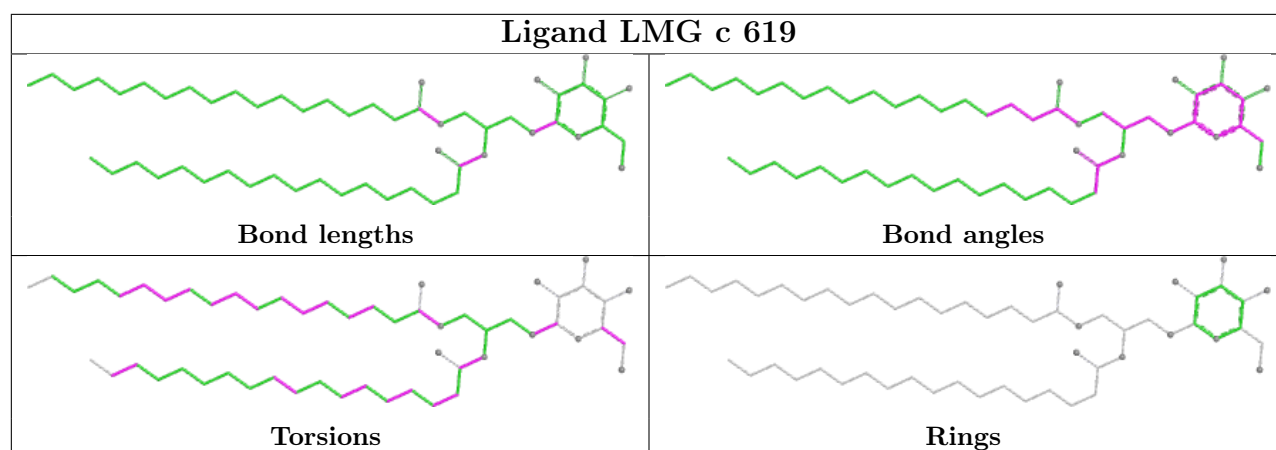
Torsions

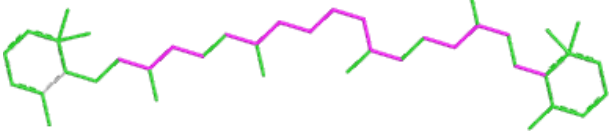
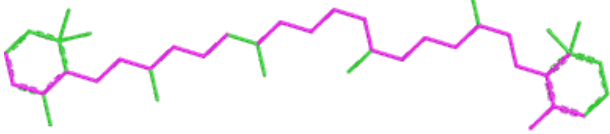
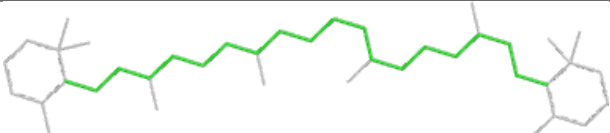
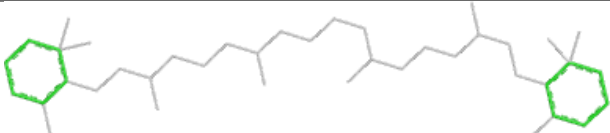
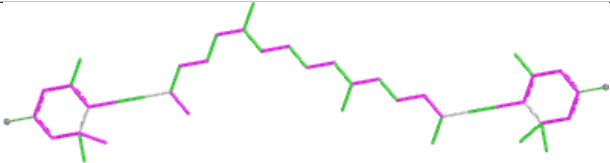
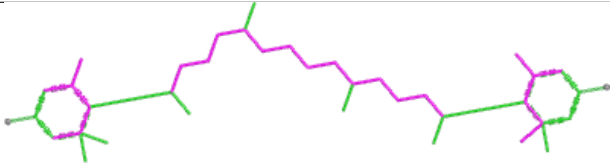
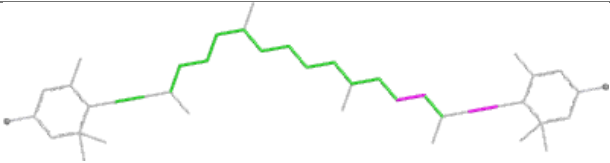
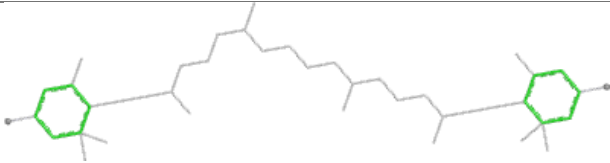
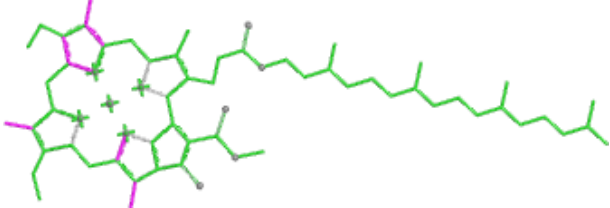
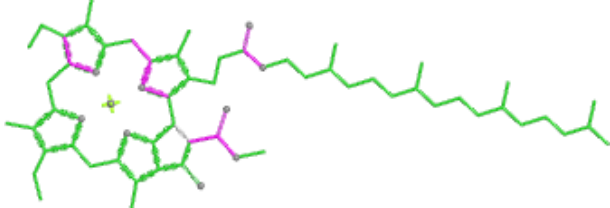
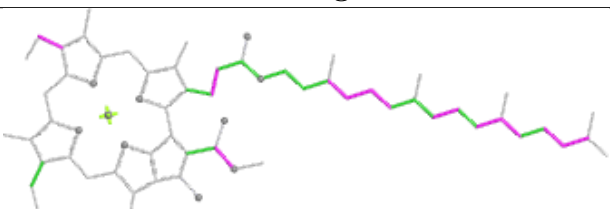
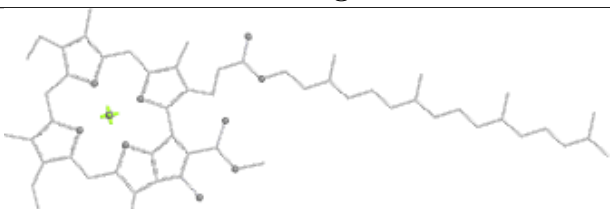


Rings



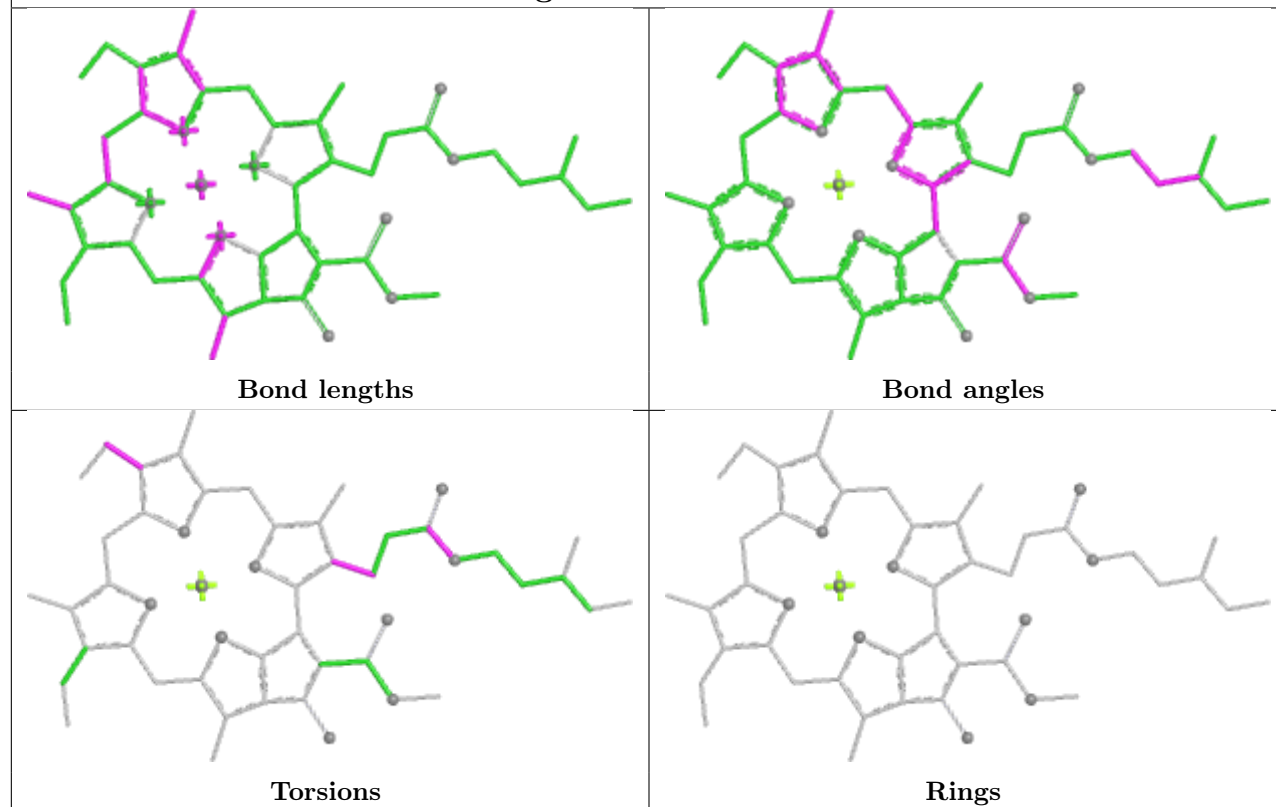




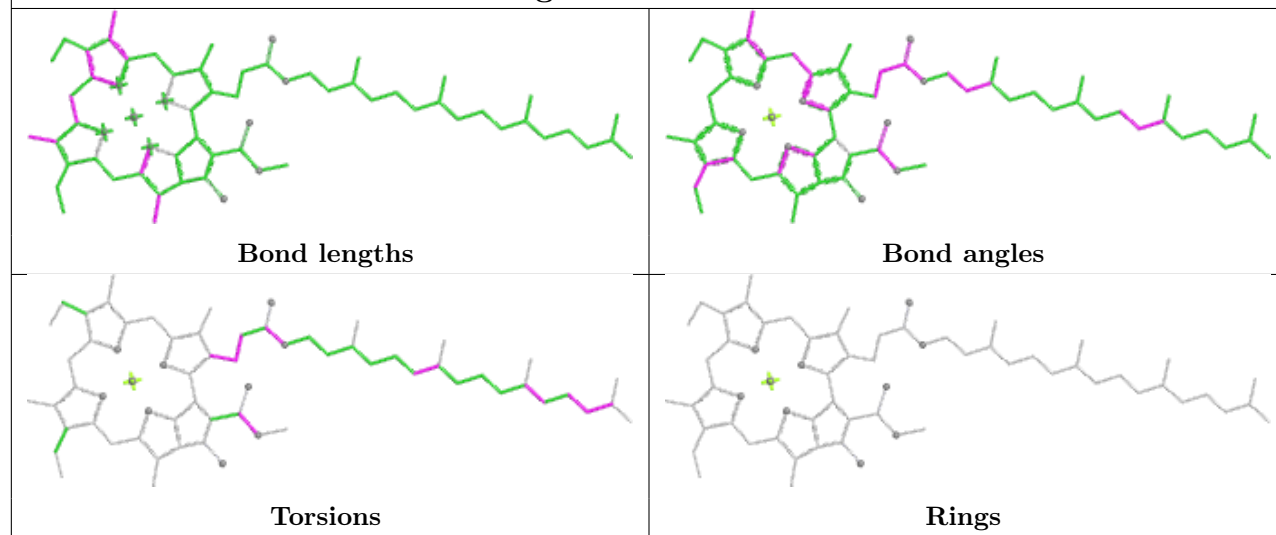
| Ligand WVN B 845                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand II0 b 613                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand CLA B 807                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

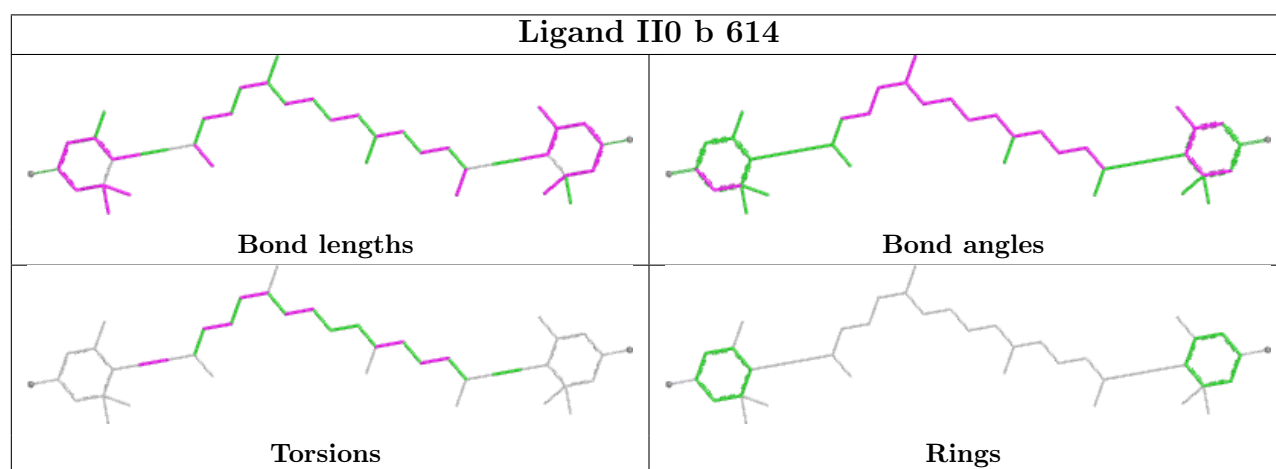
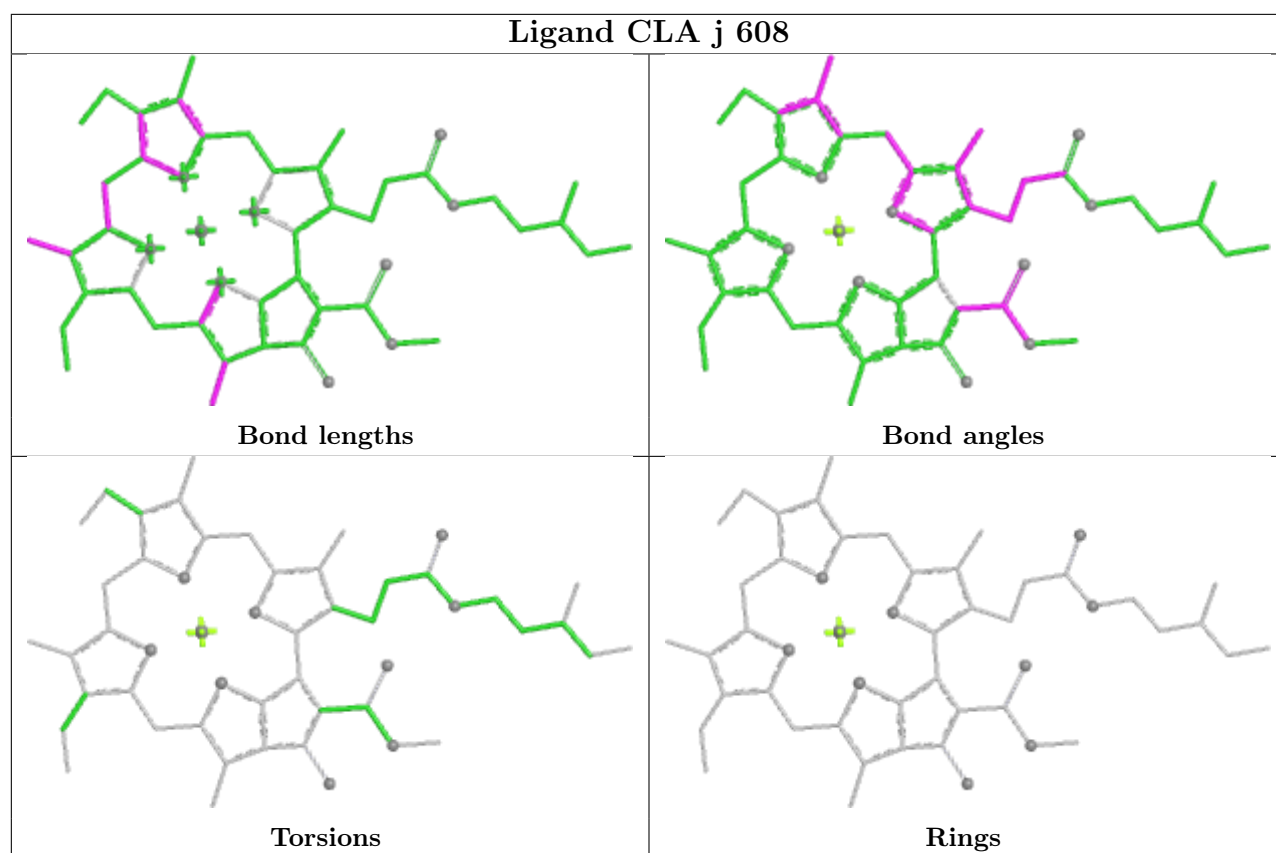


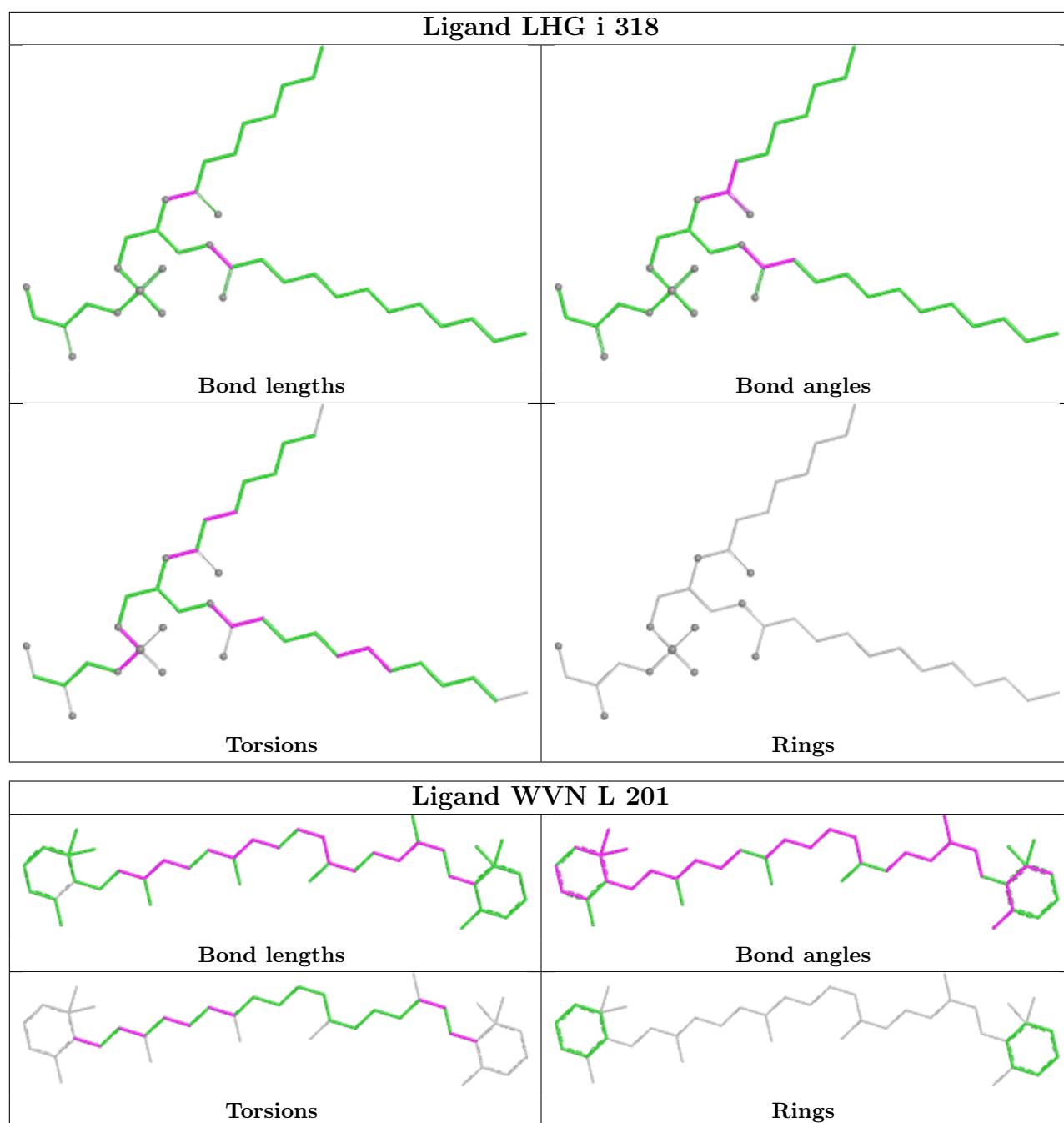
## Ligand CLA b 612

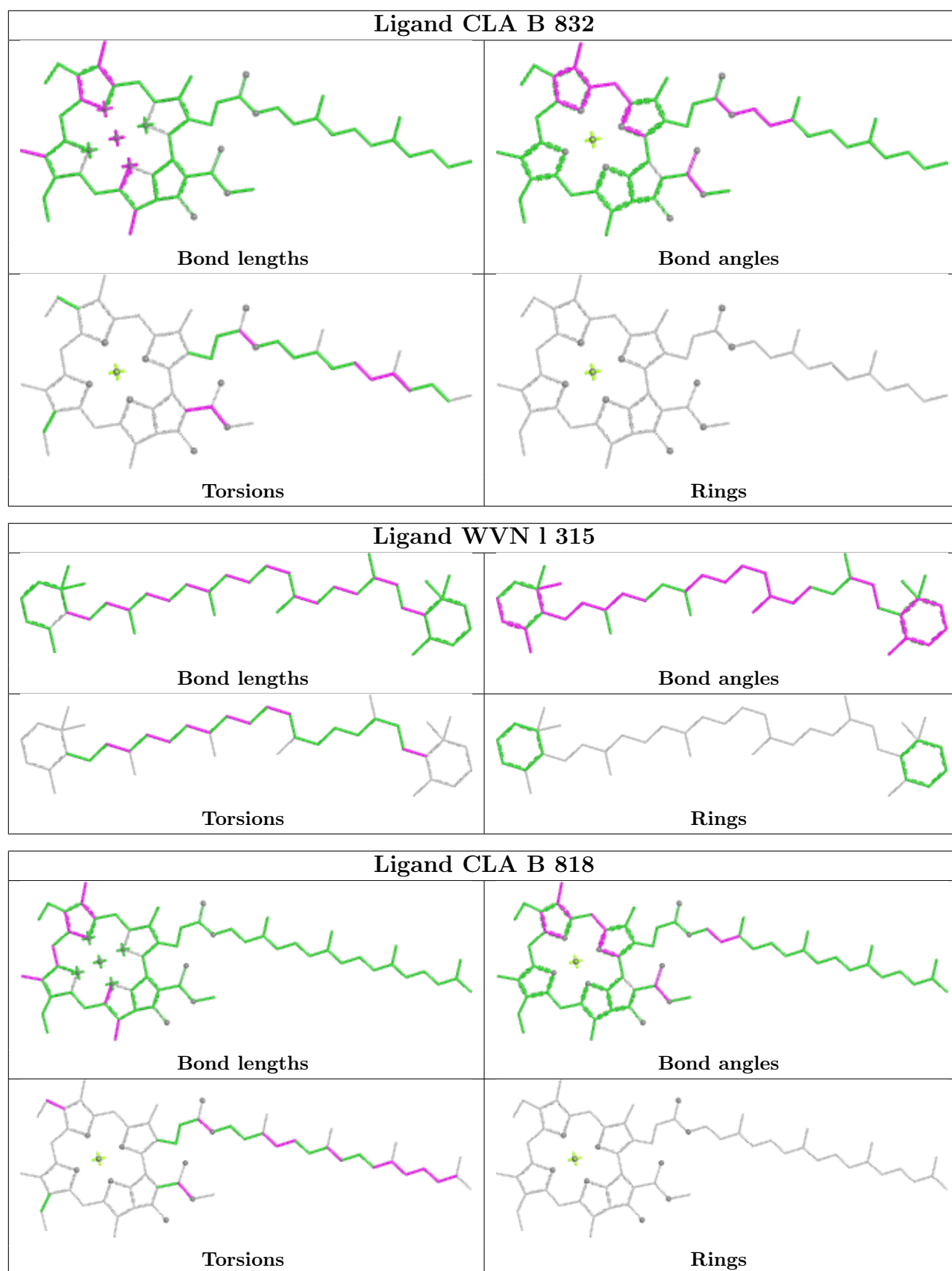


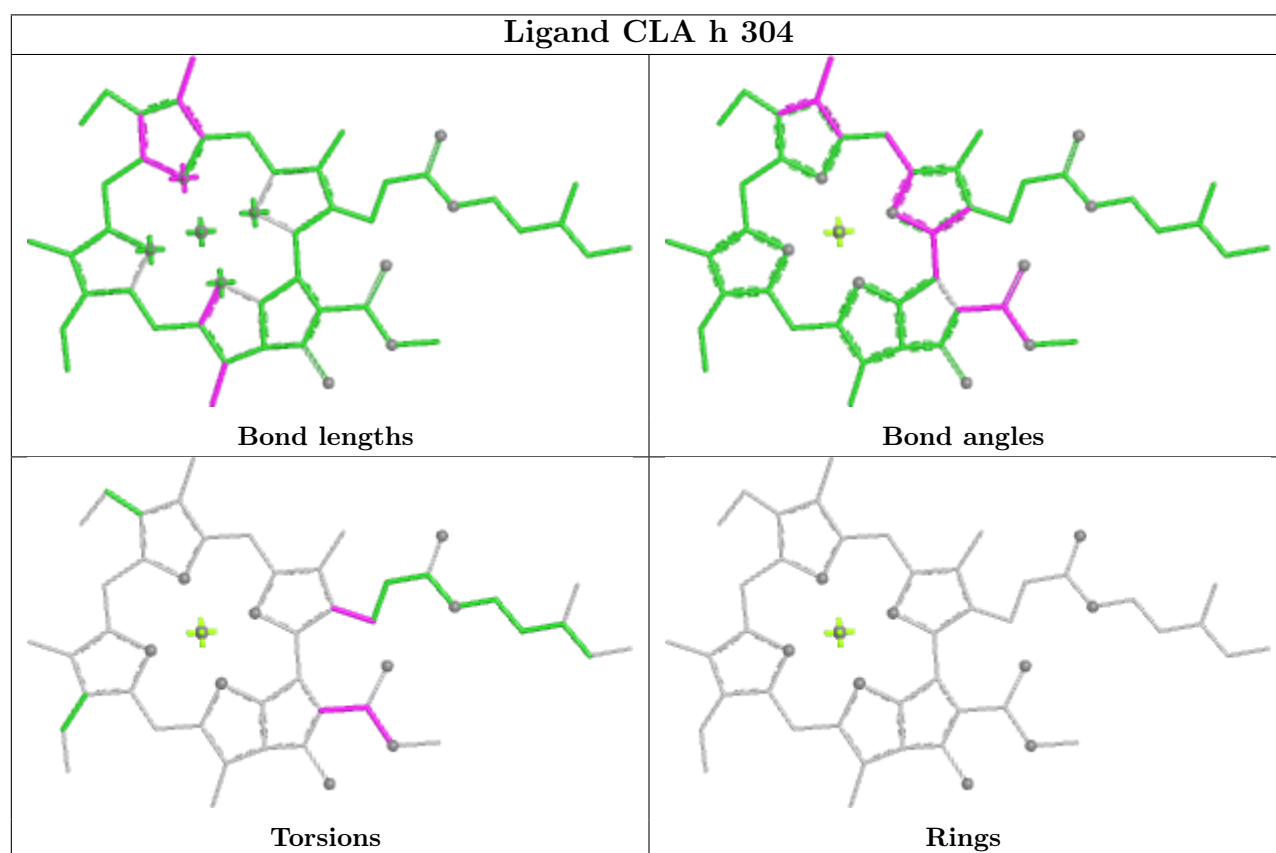
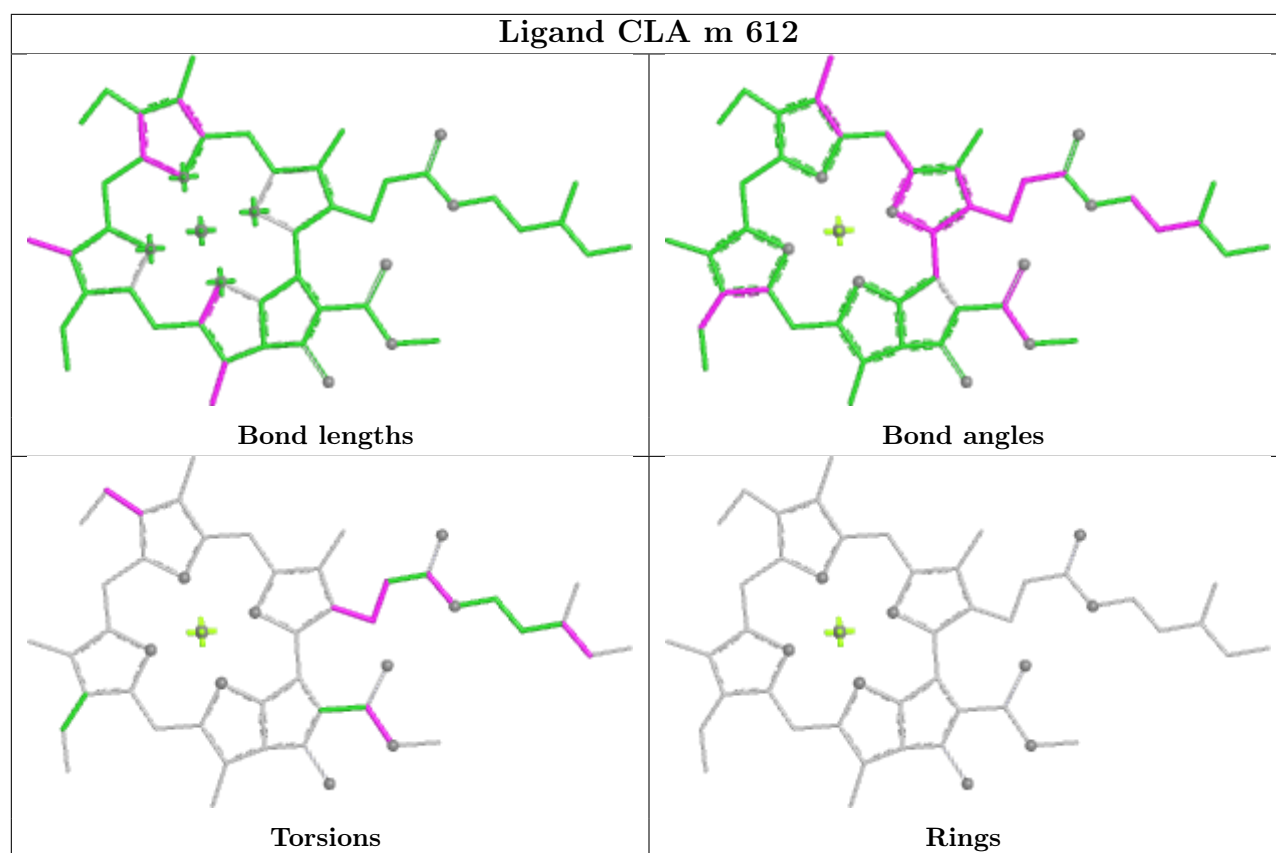
## Ligand CLA k 609



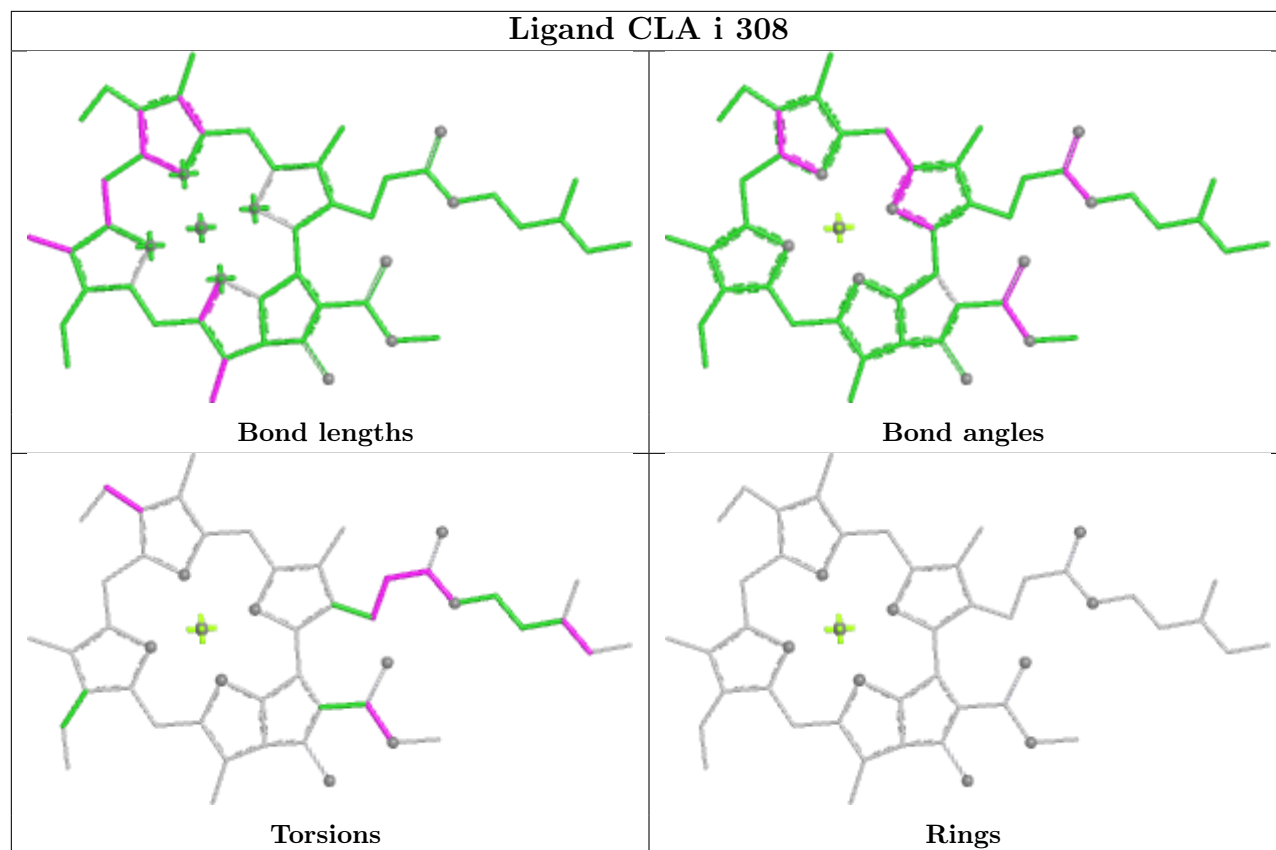




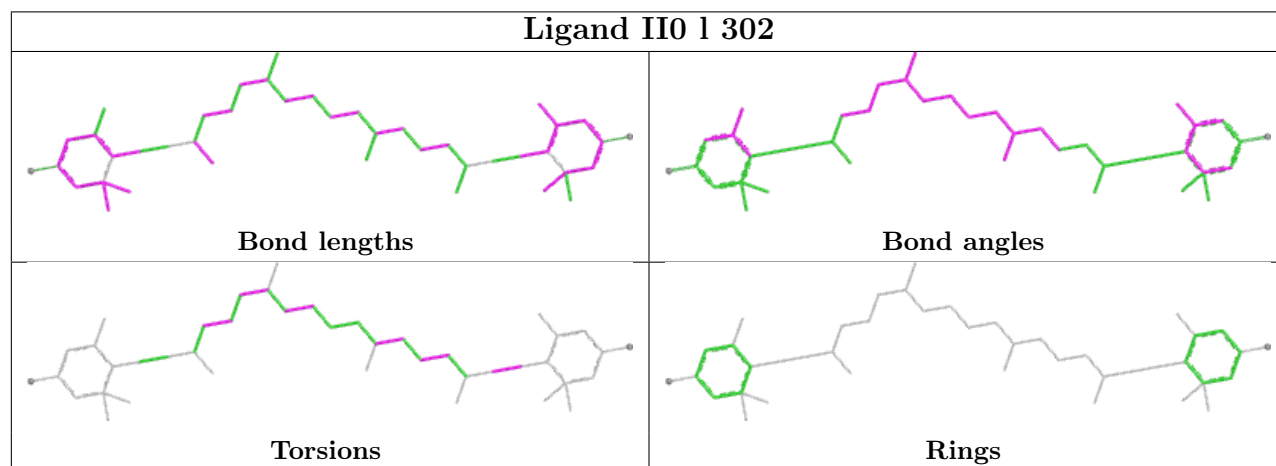


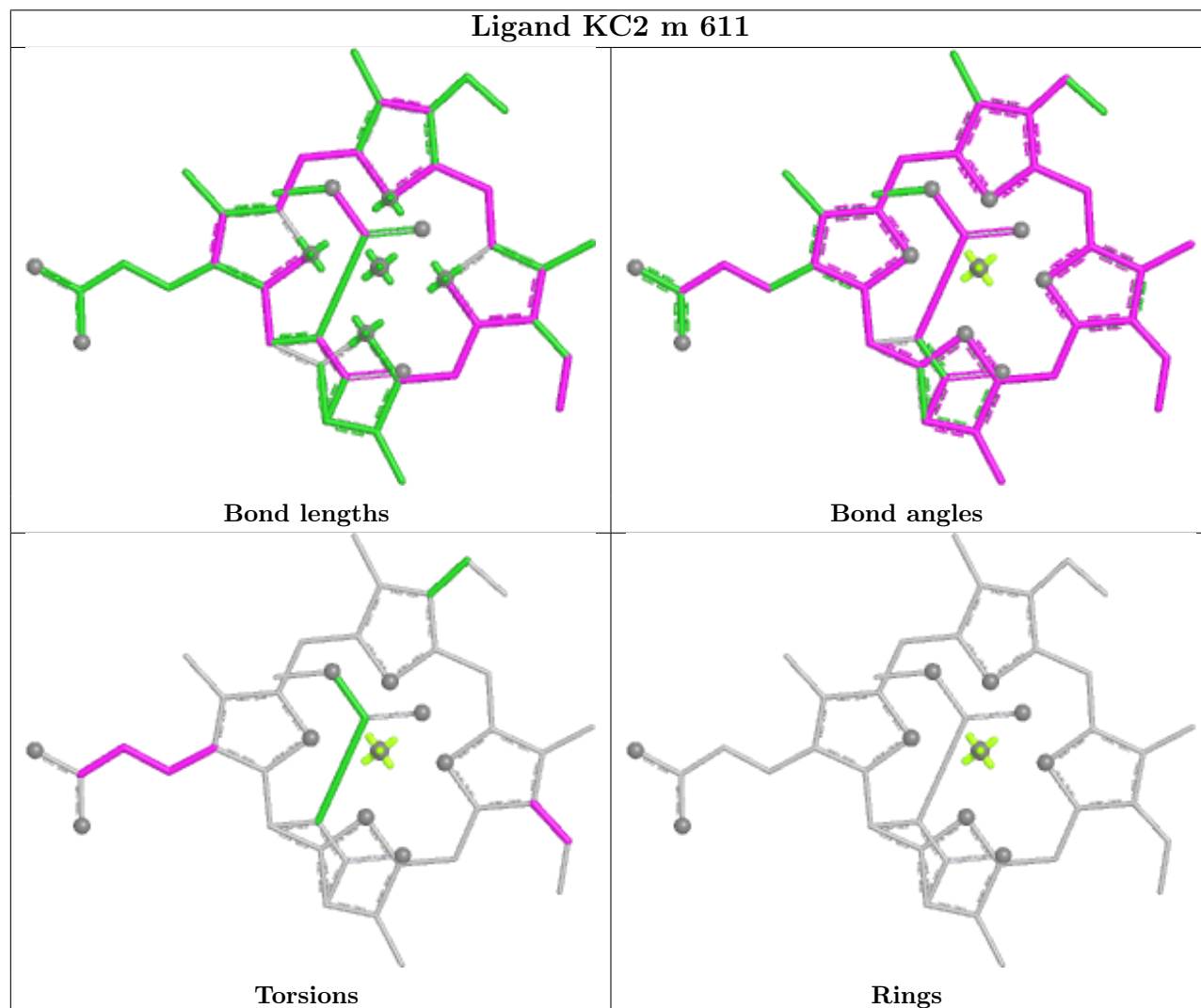
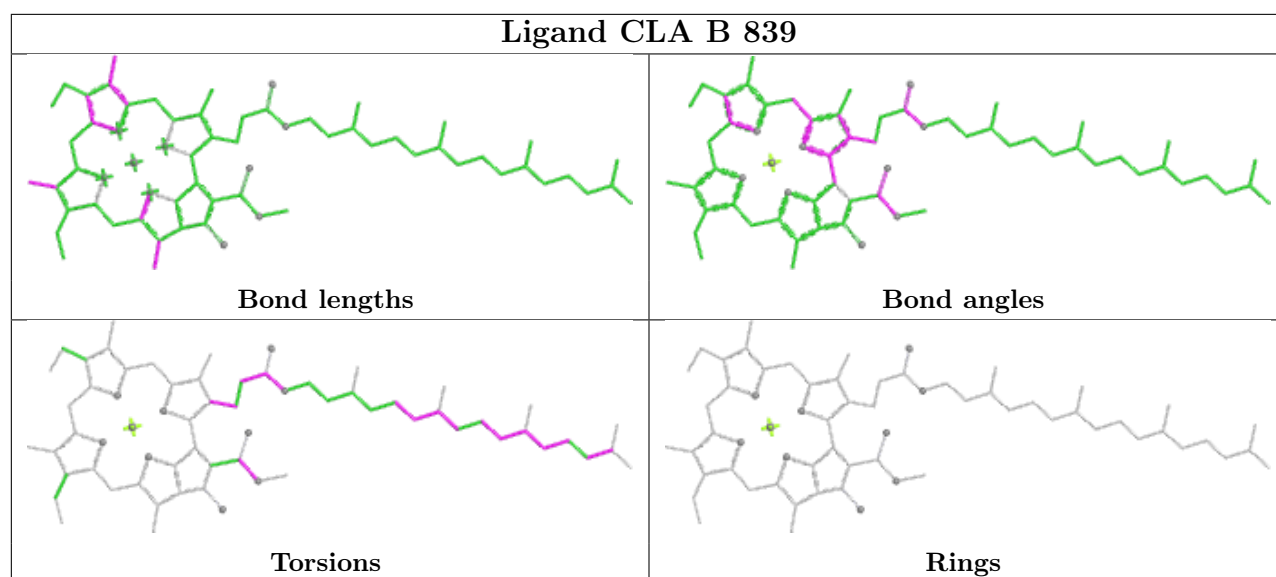


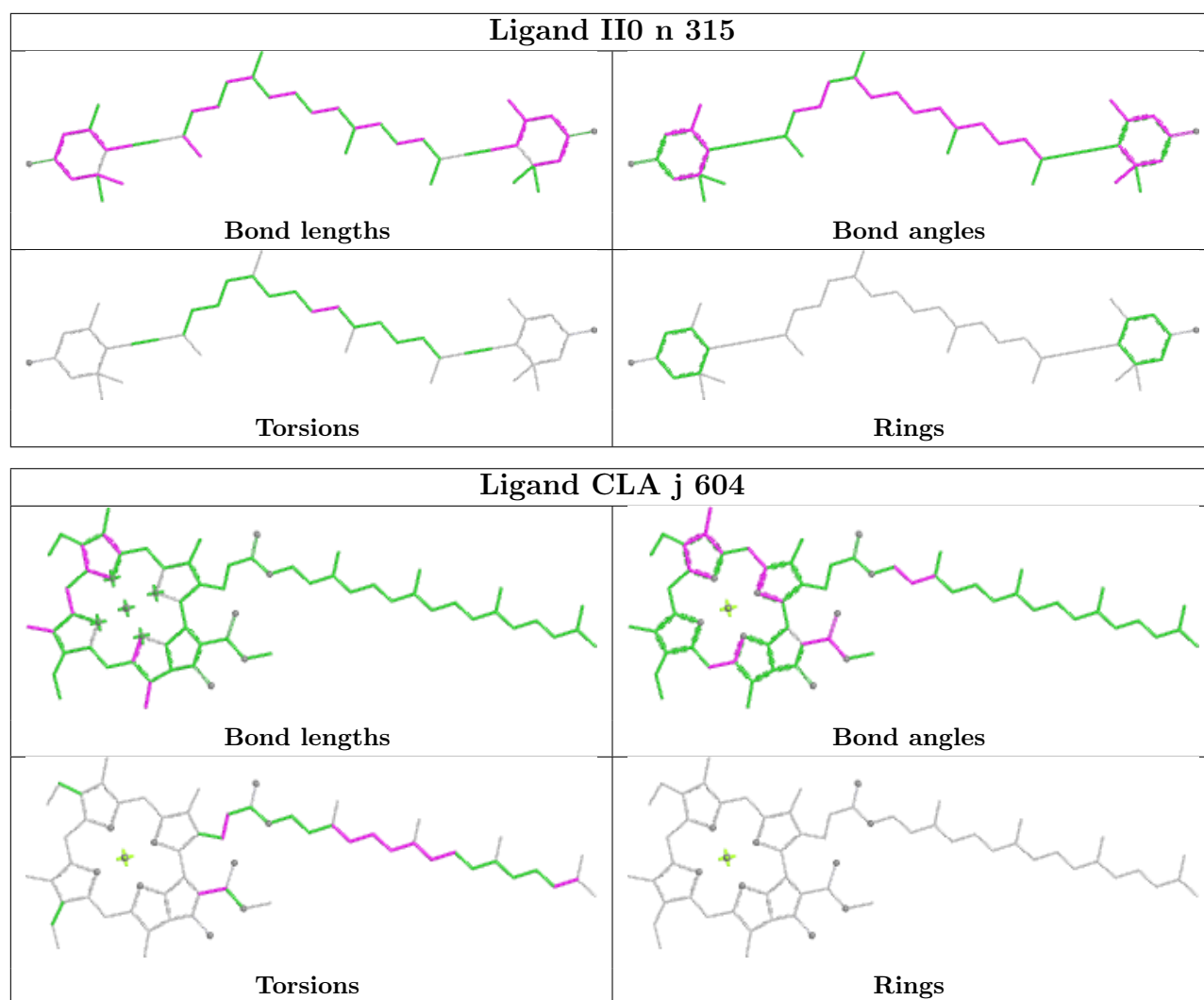
## Ligand CLA i 308



## Ligand II0 l 302

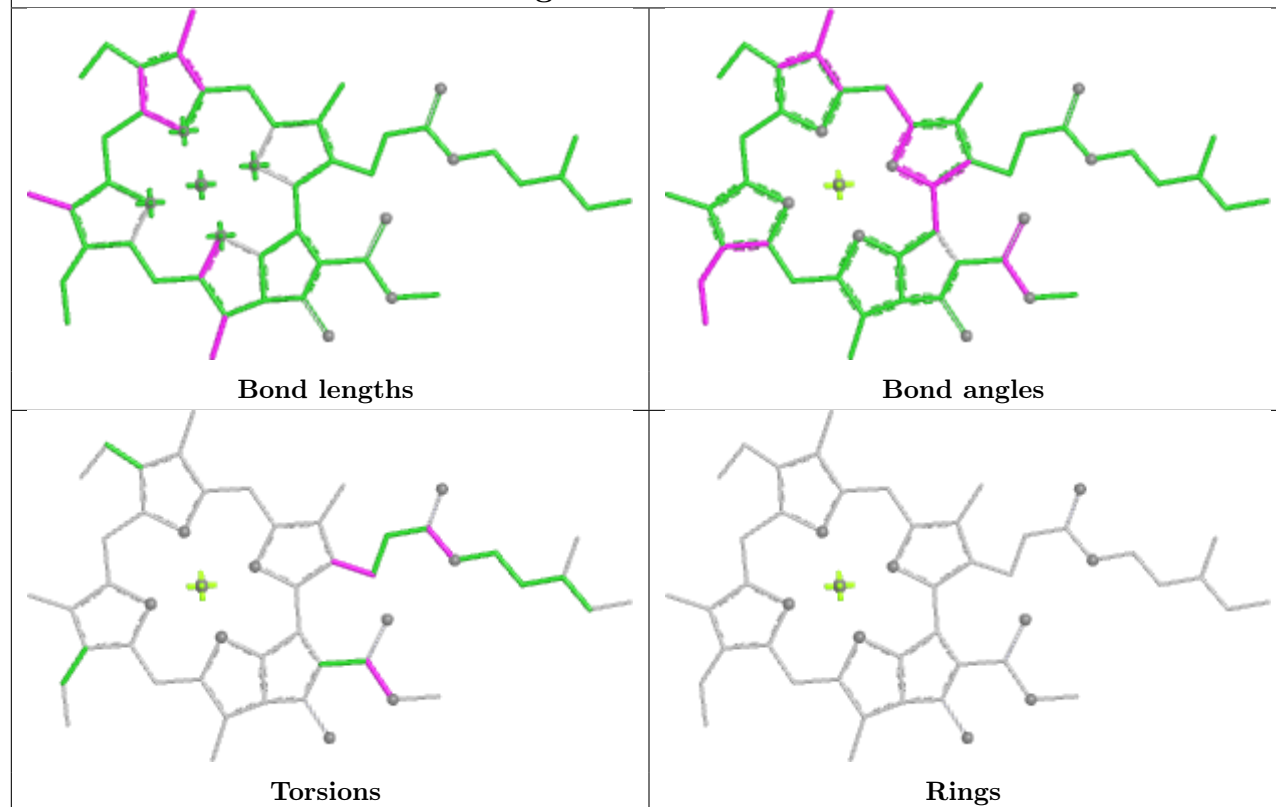




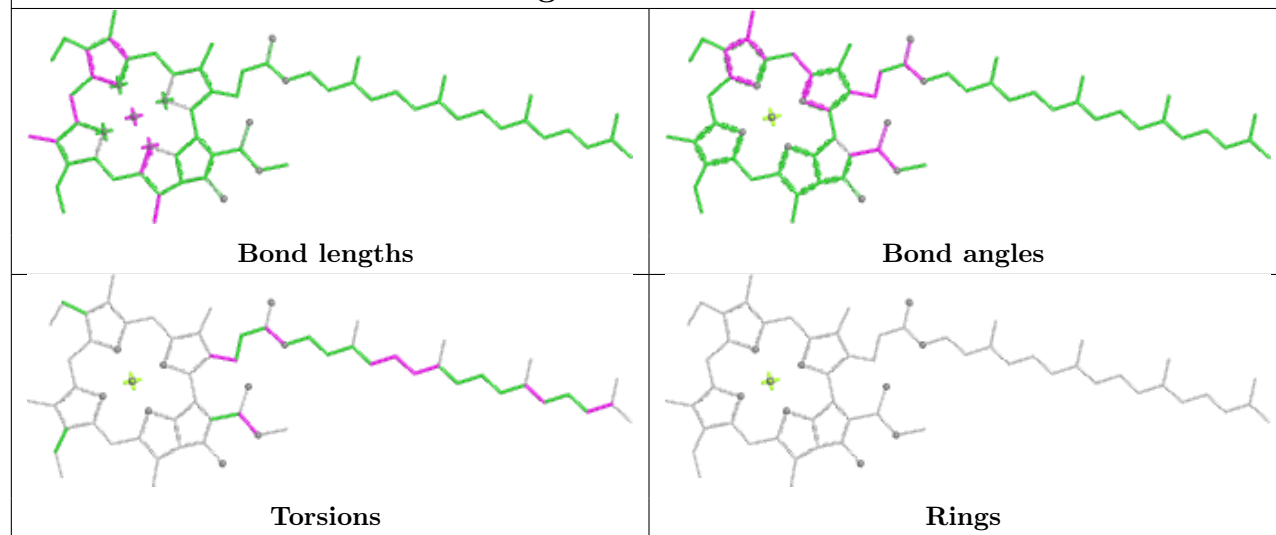




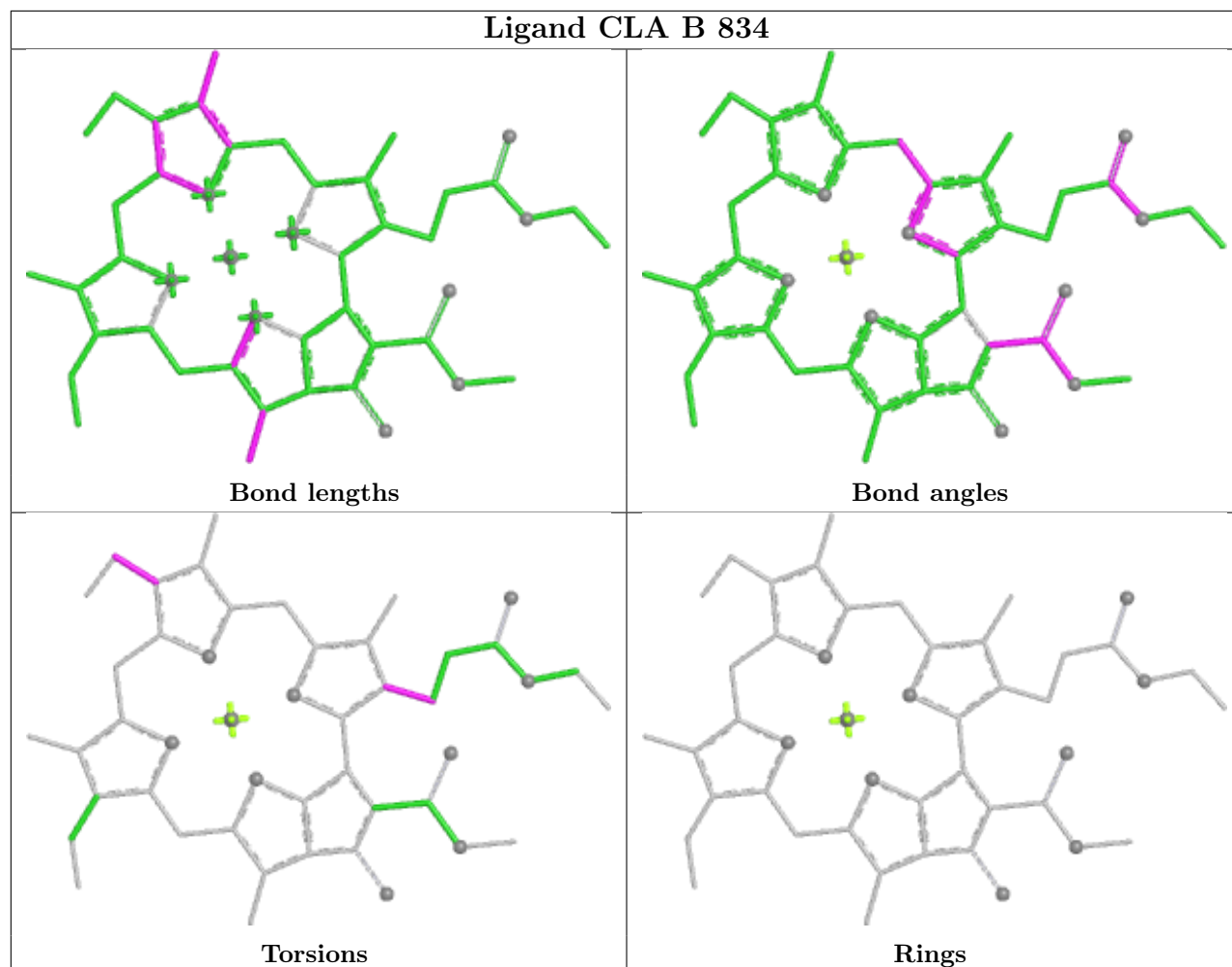
## Ligand CLA n 306



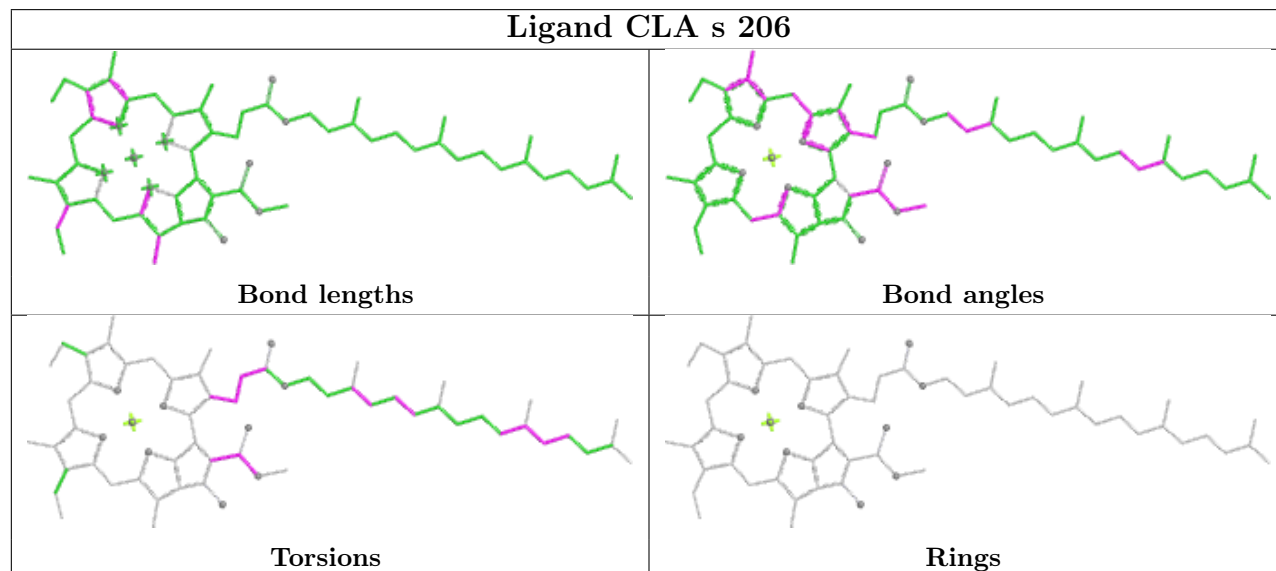
## Ligand CLA s 203

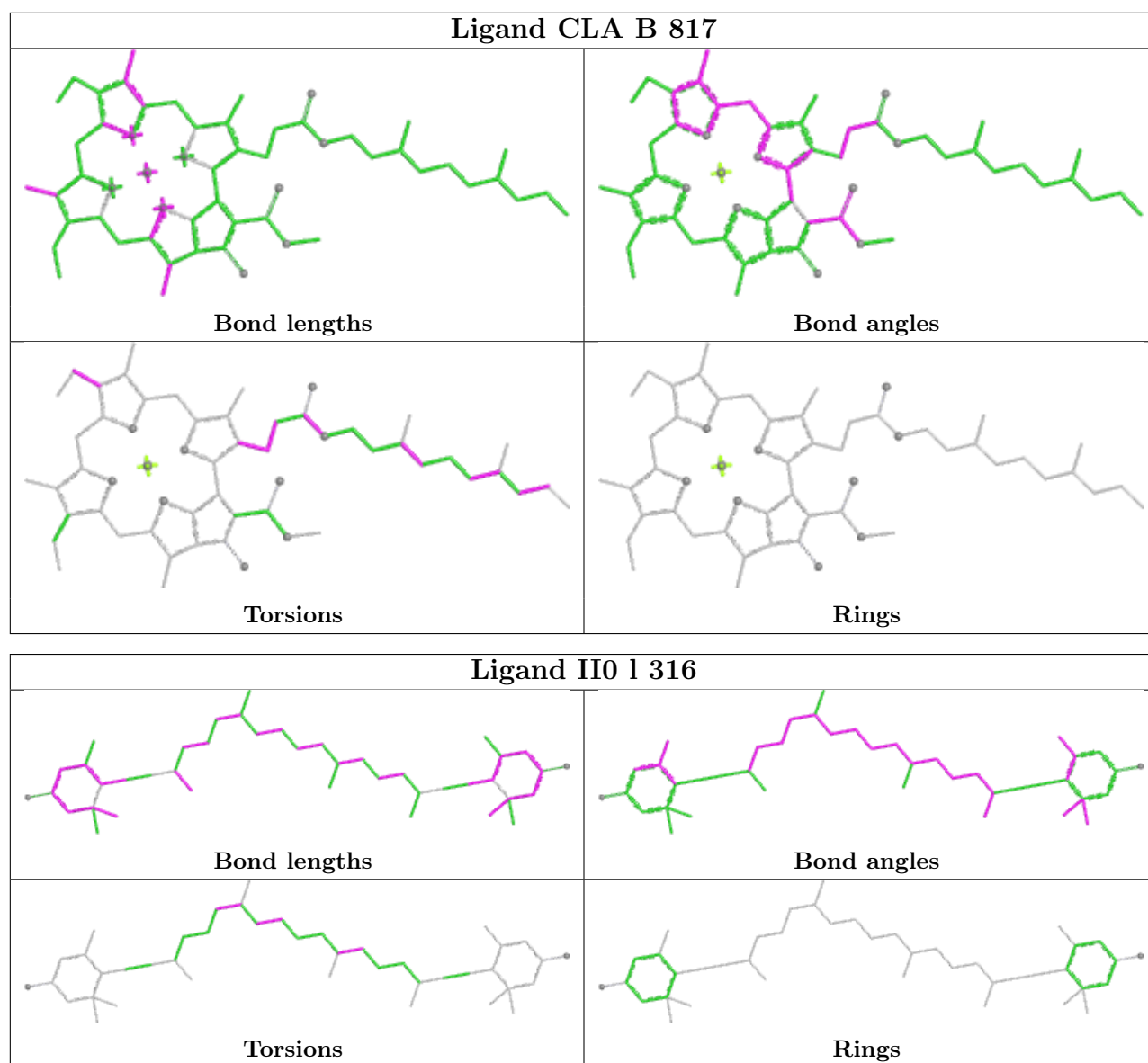


## Ligand CLA B 834

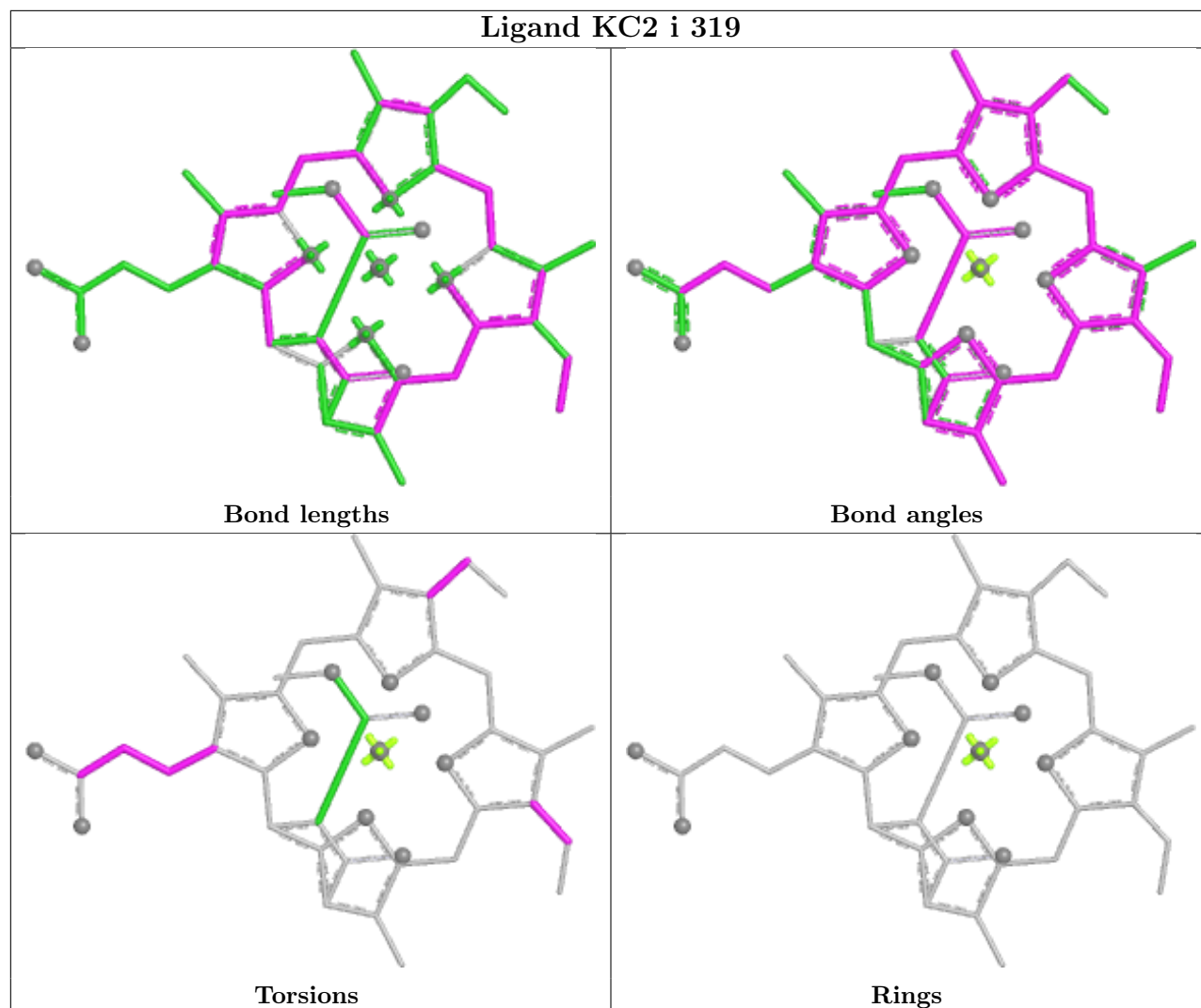


## Ligand CLA s 206

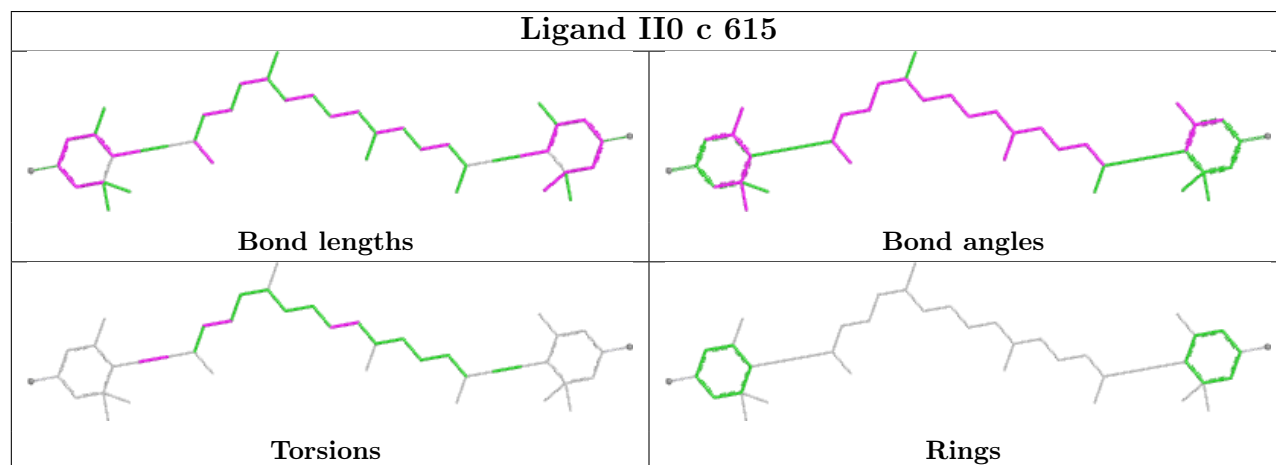




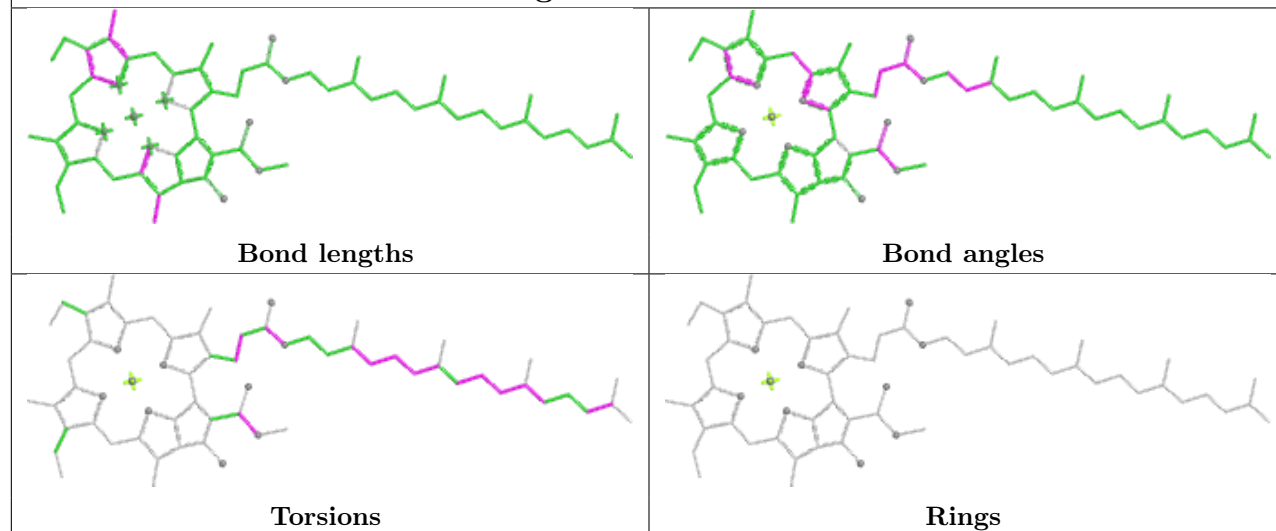
## Ligand KC2 i 319



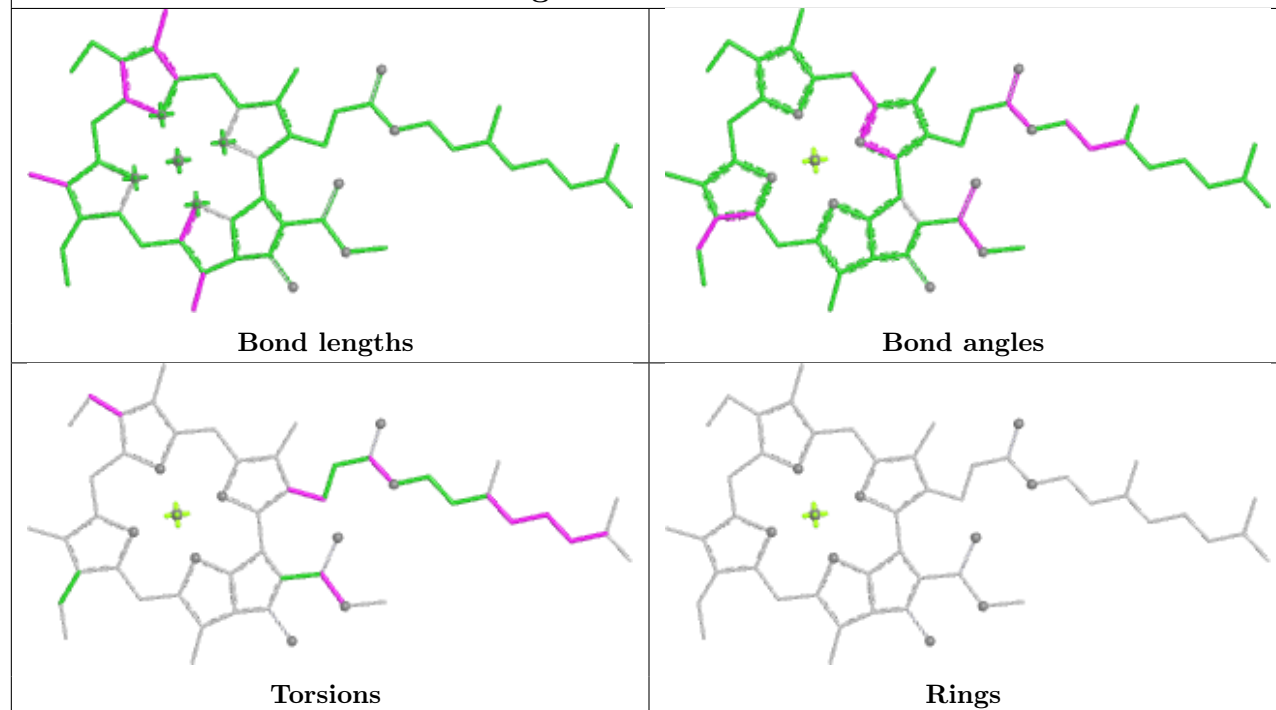
## Ligand II0 c 615

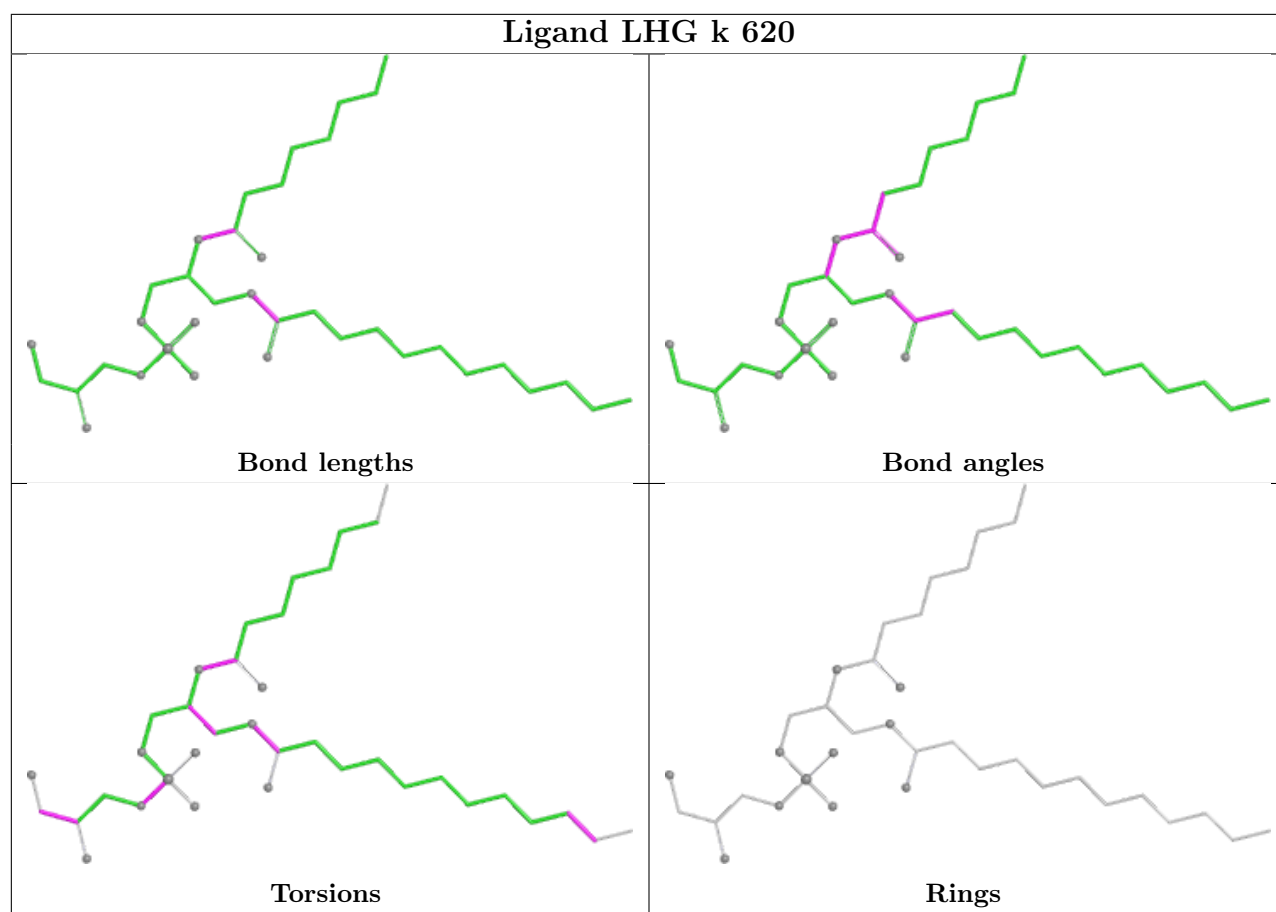


## Ligand CLA b 611

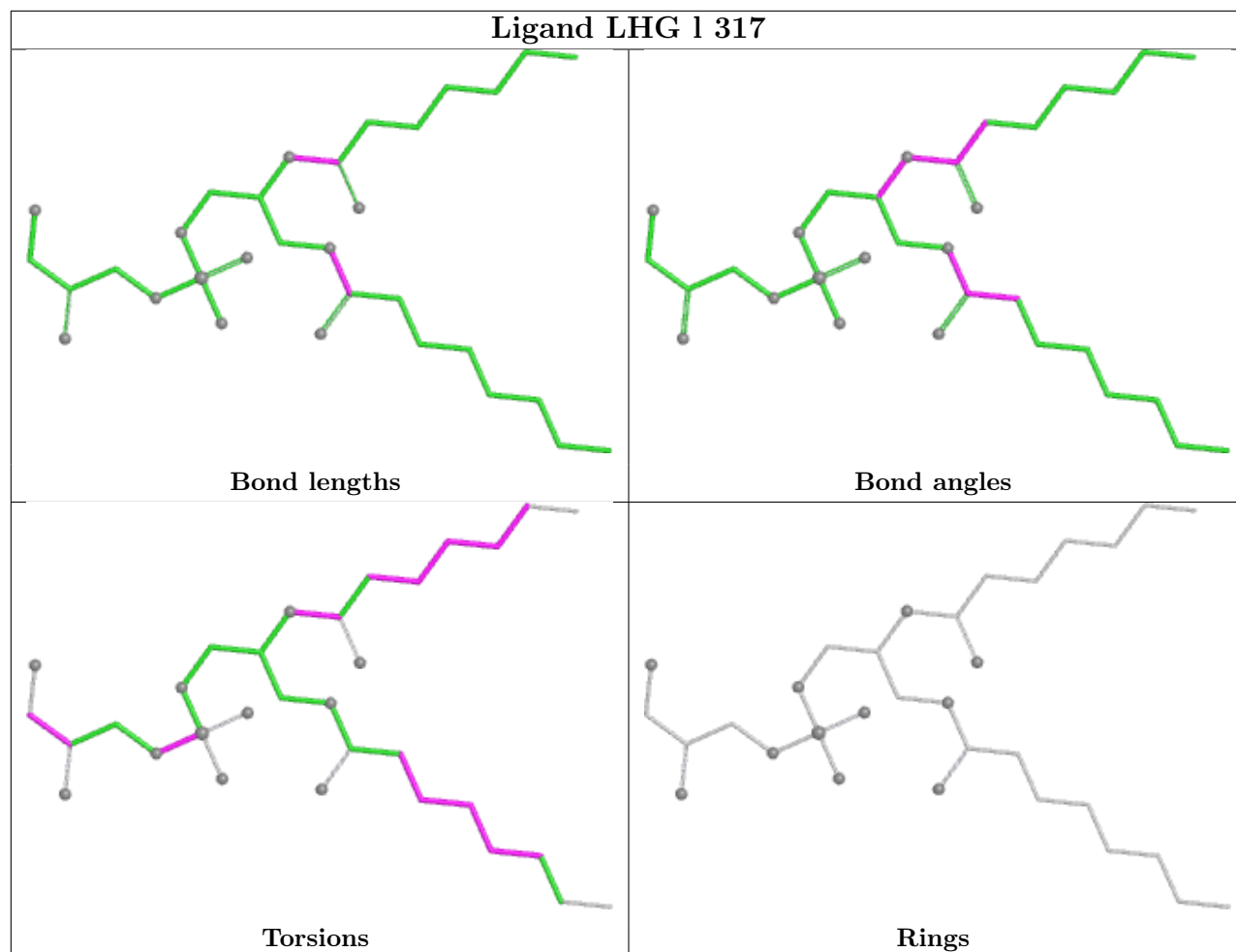


## Ligand CLA A 823

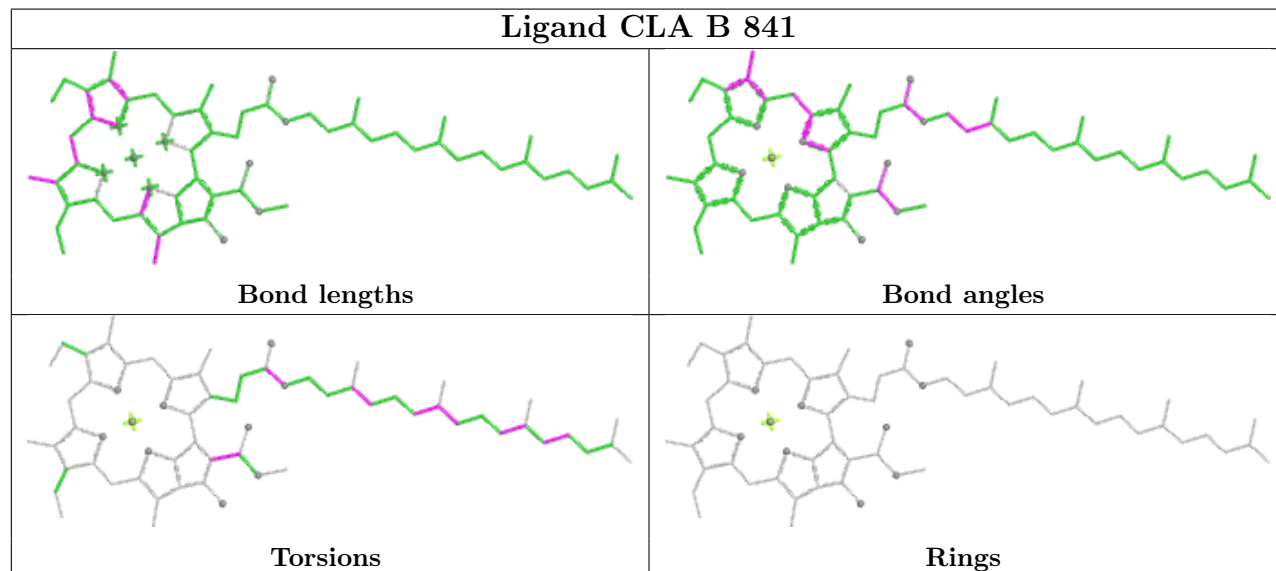




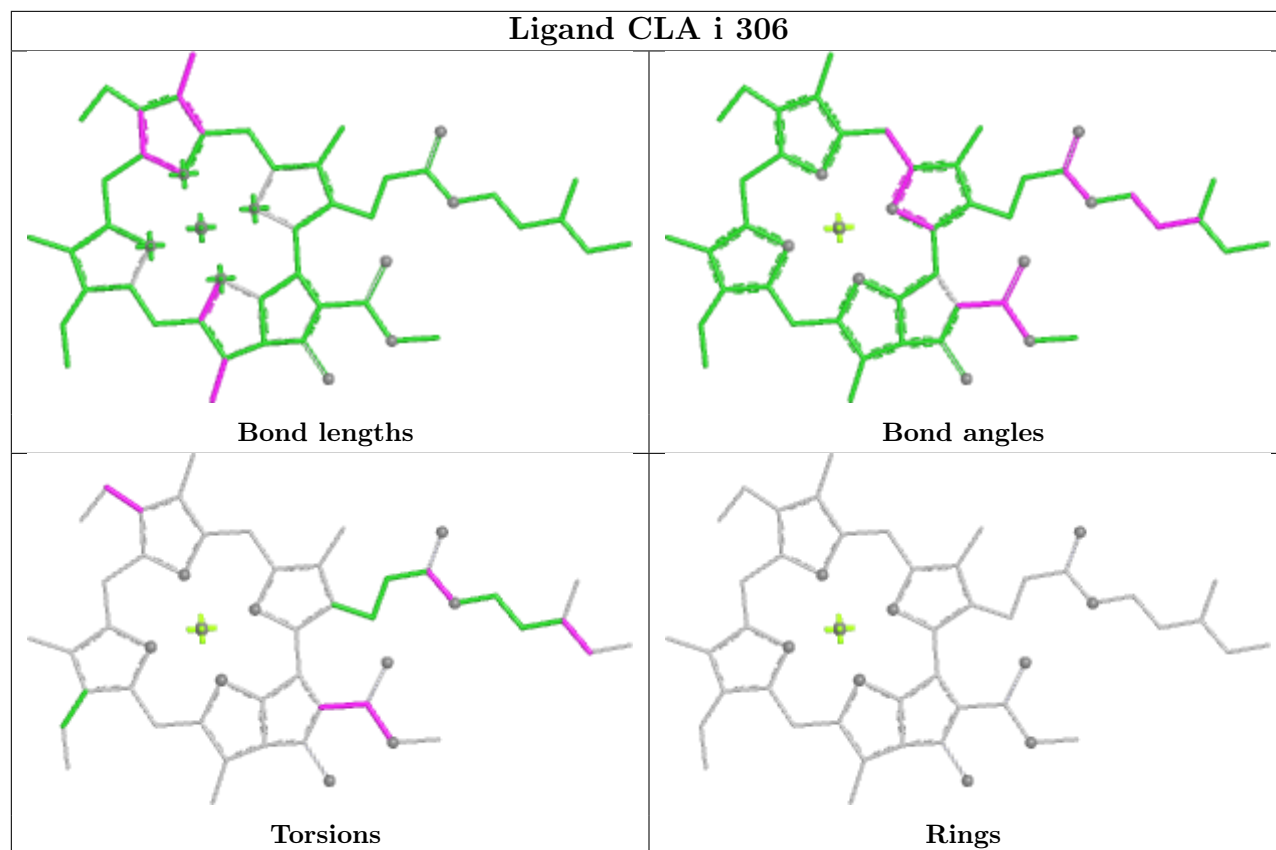
## Ligand LHG 1 317



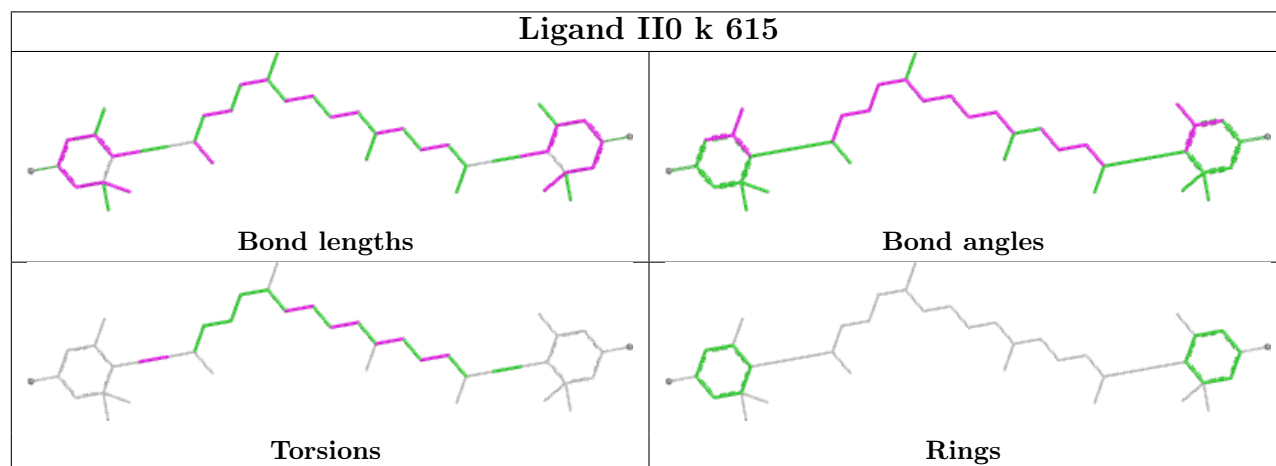
## Ligand CLA B 841



## Ligand CLA i 306

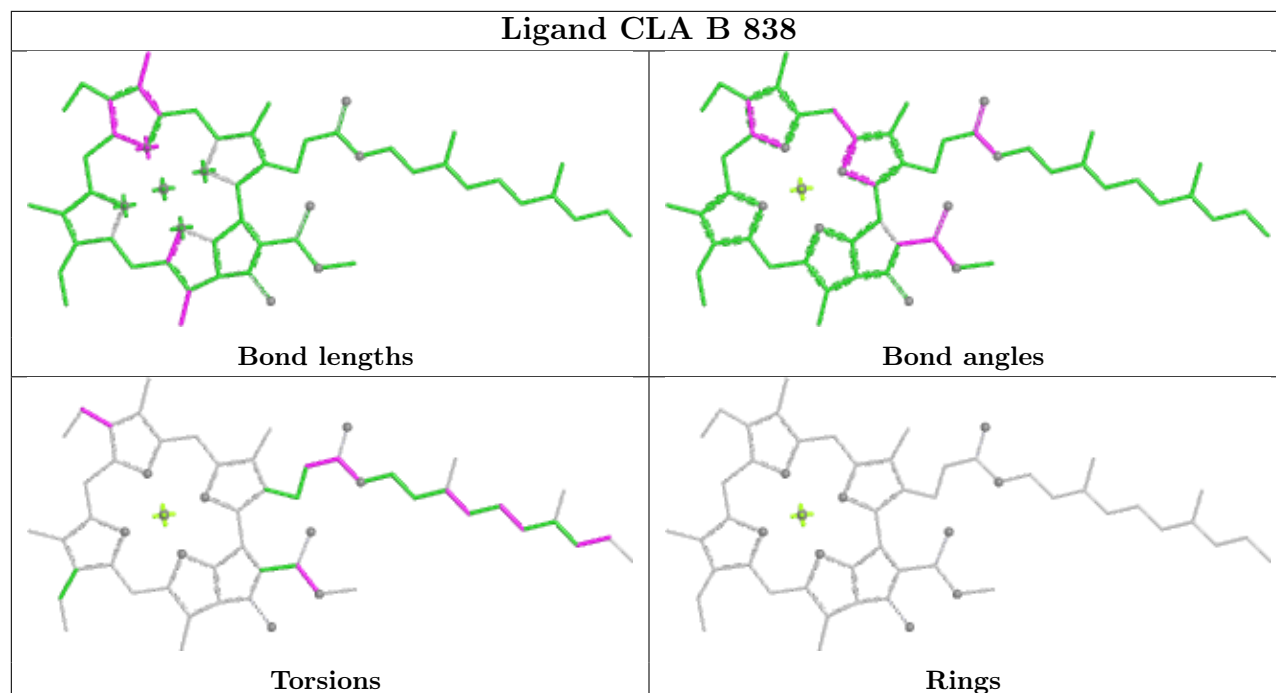


## Ligand II0 k 615

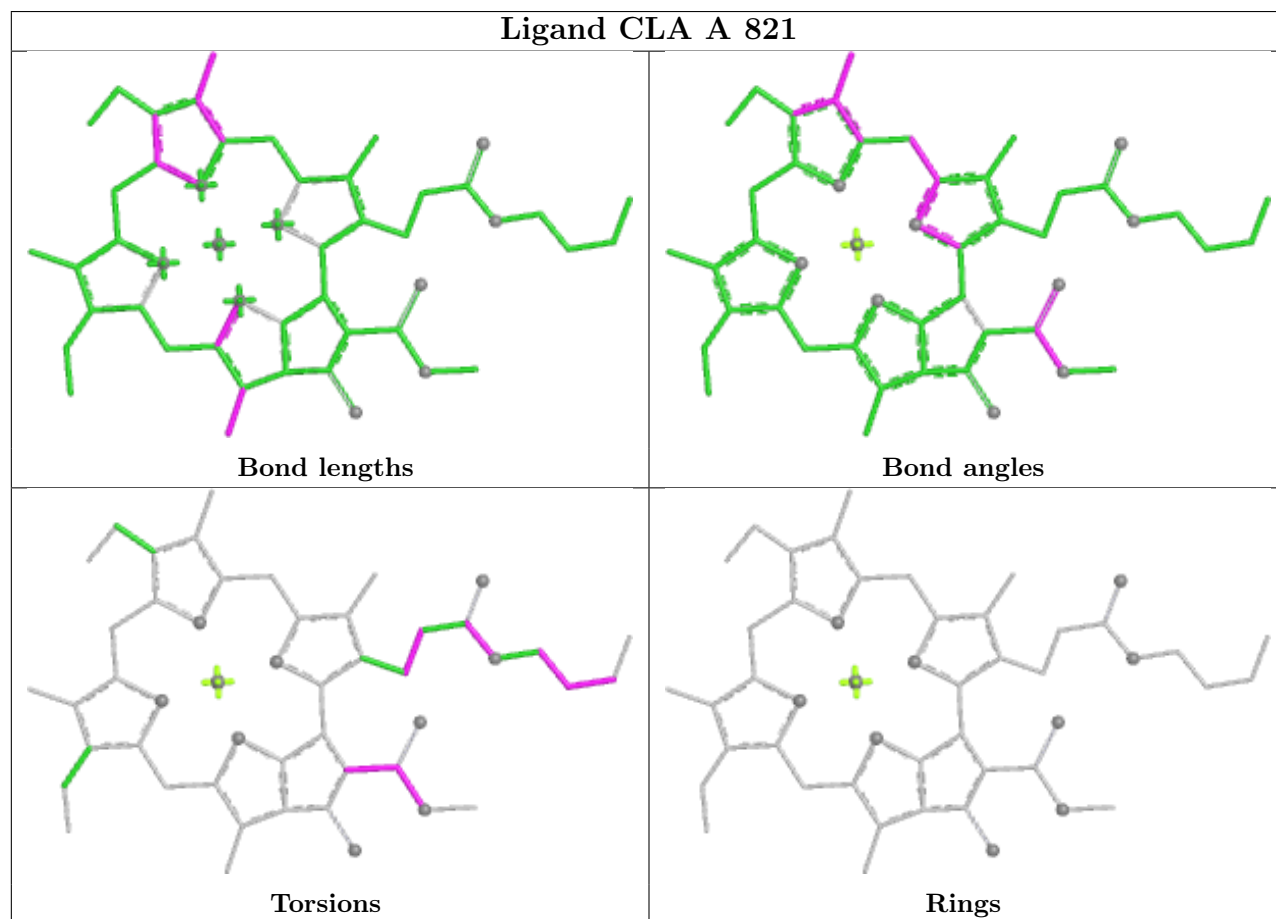




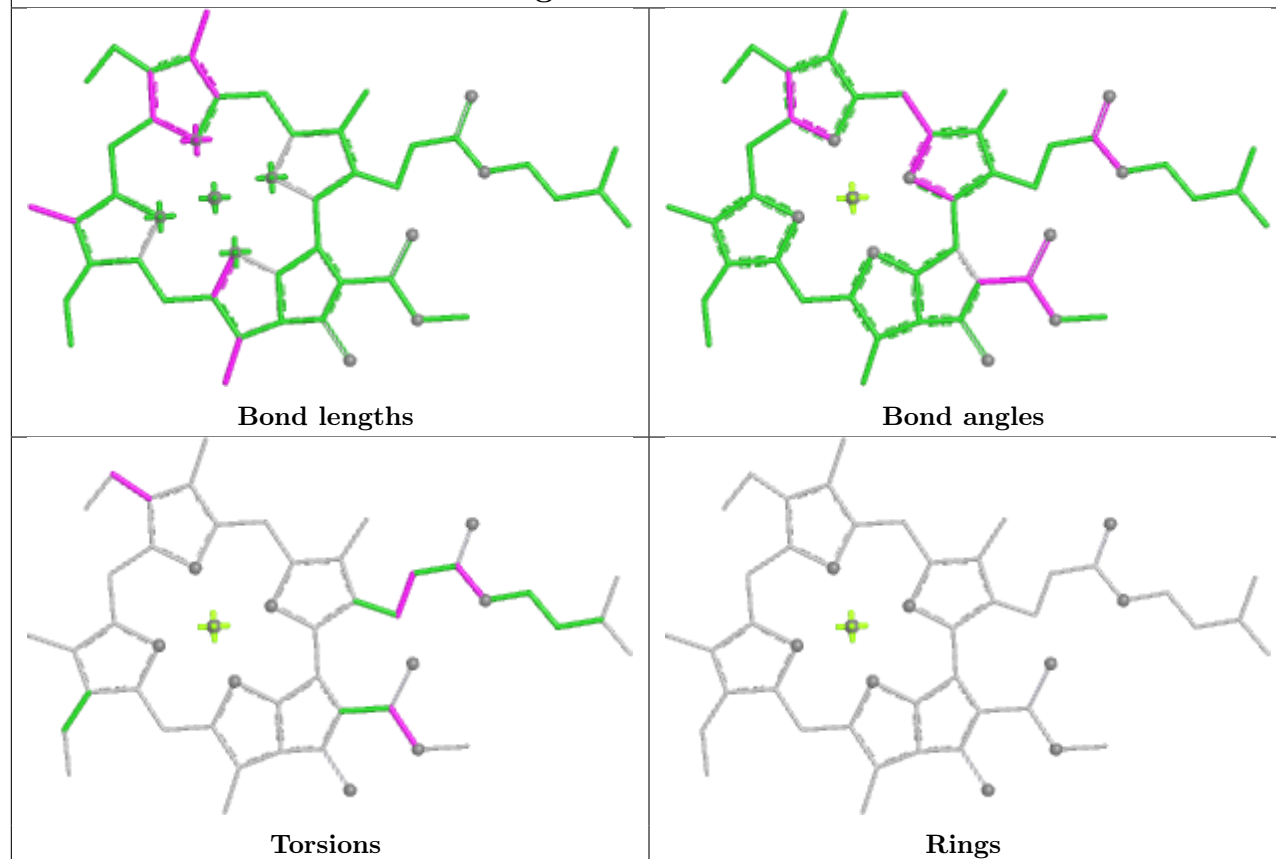
## Ligand CLA B 838



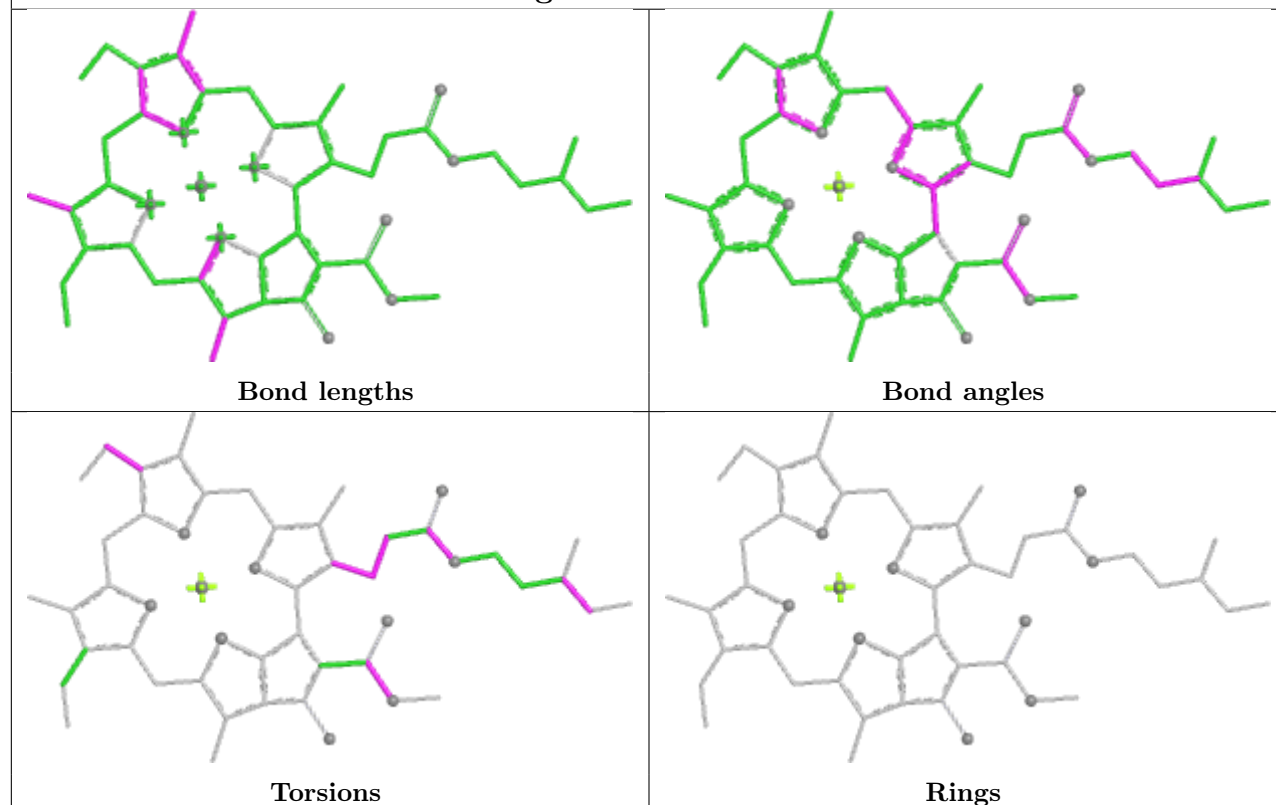
## Ligand CLA A 821

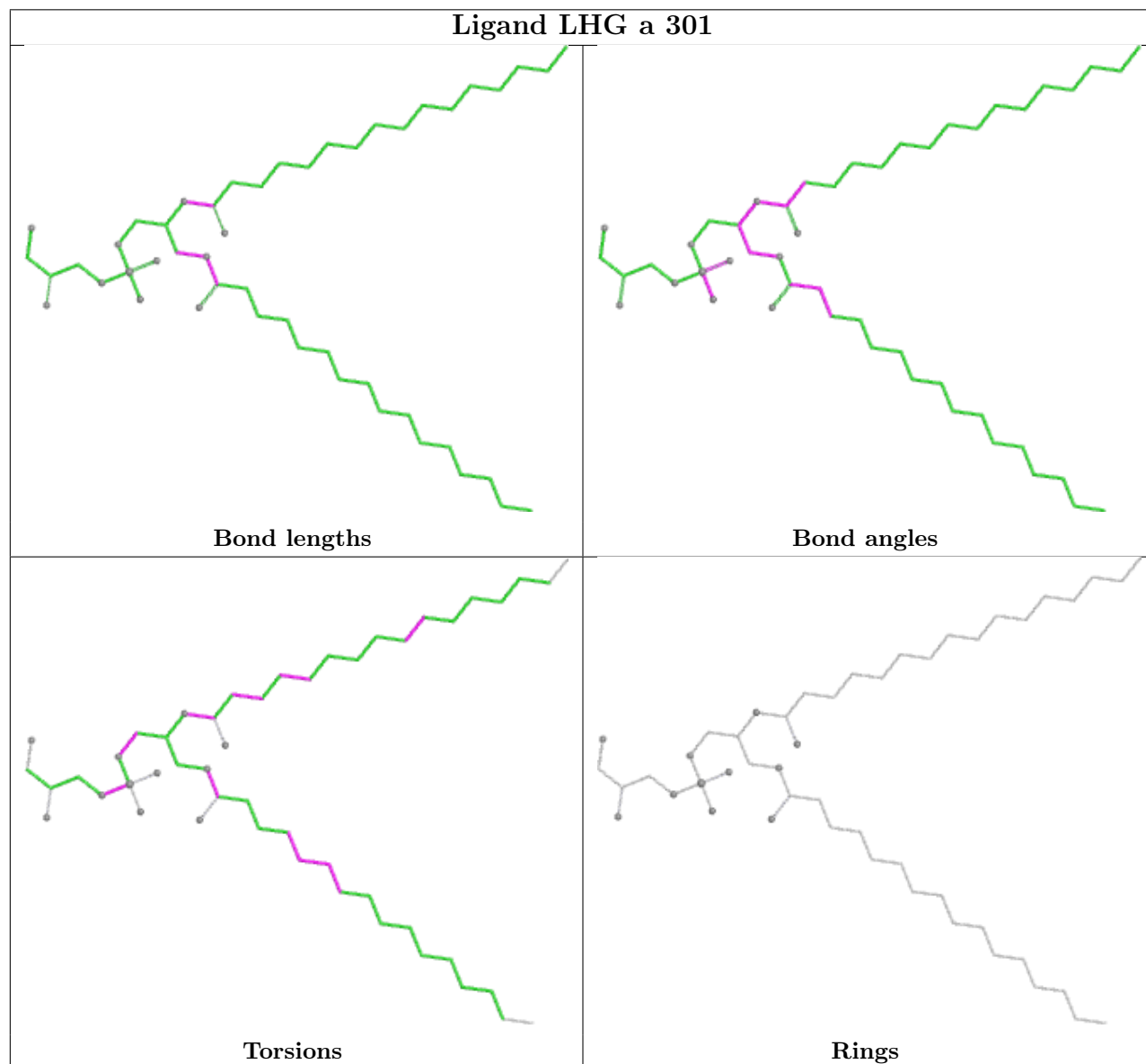
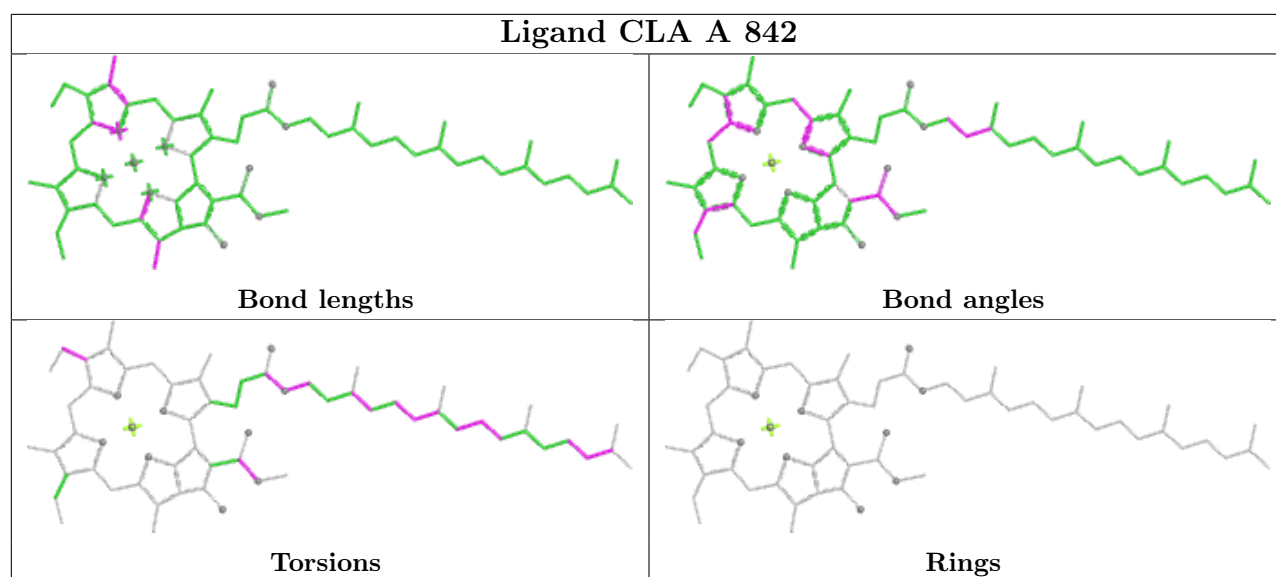


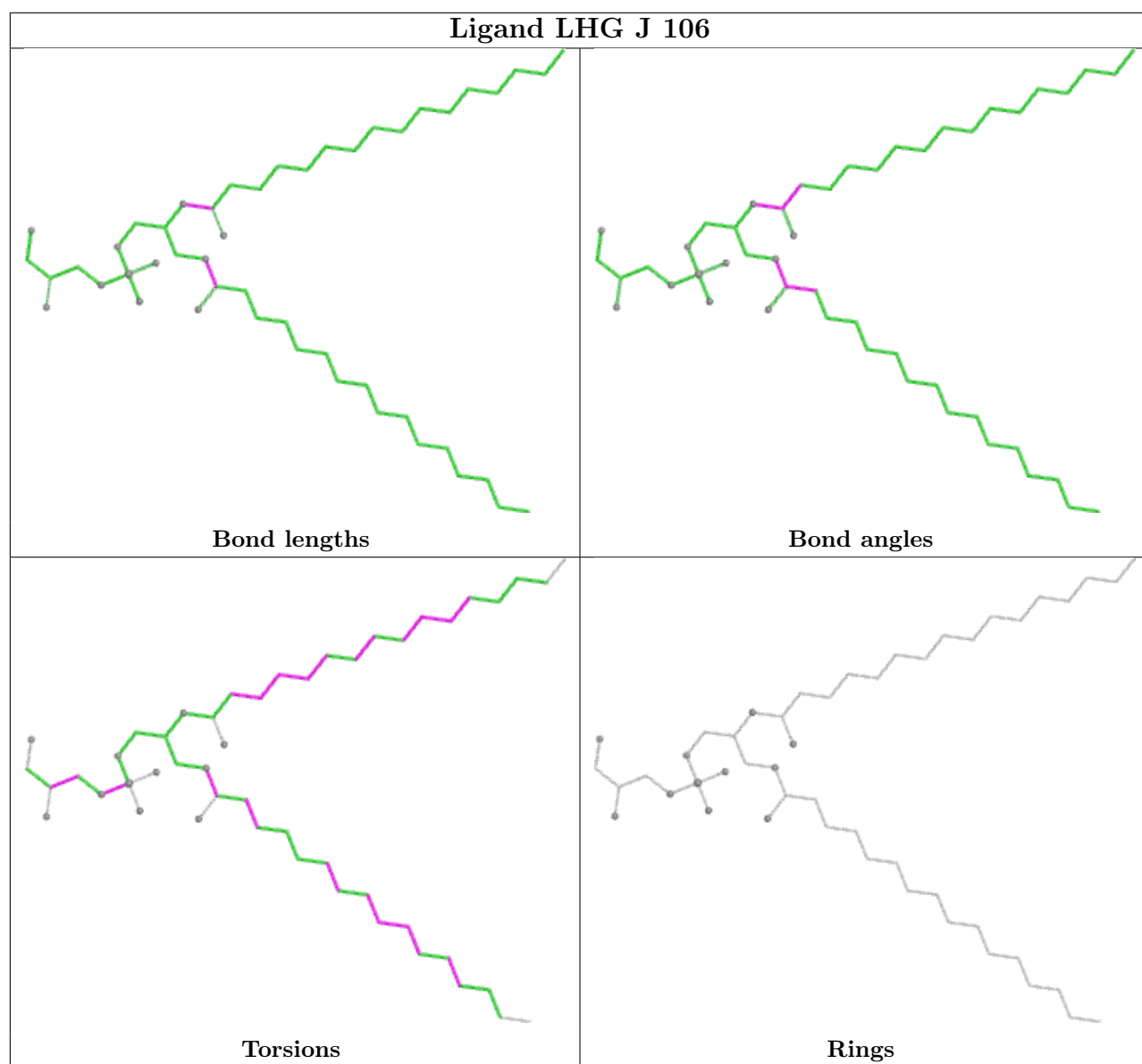
## Ligand CLA n 303



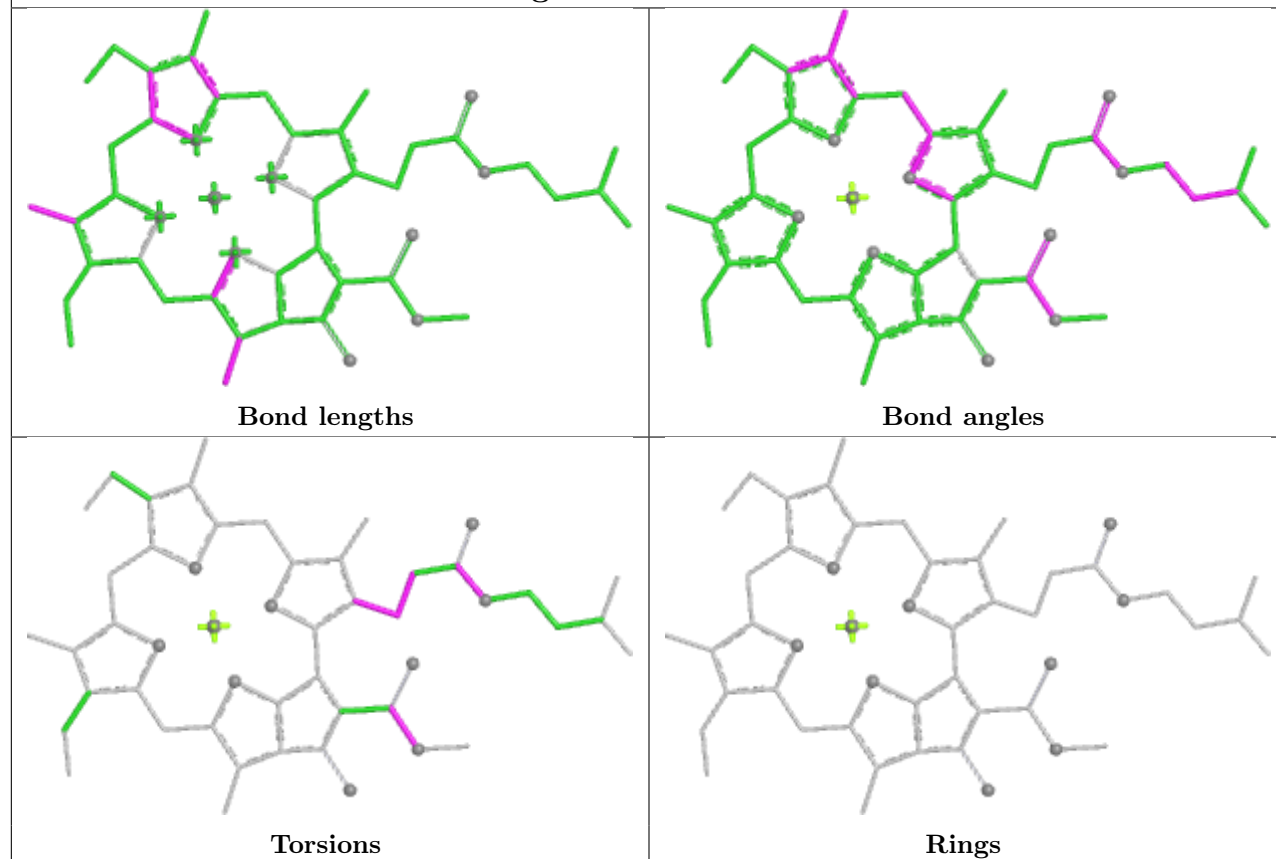
## Ligand CLA n 314



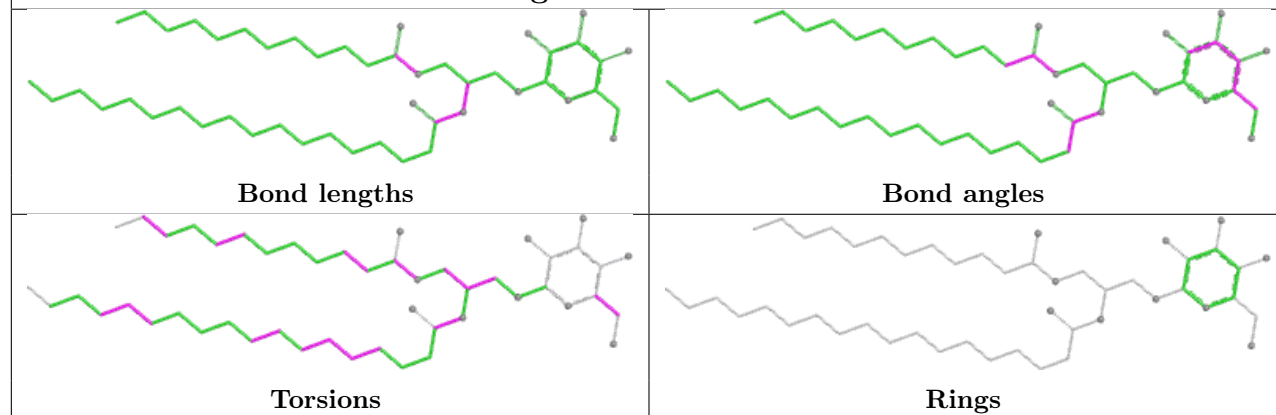




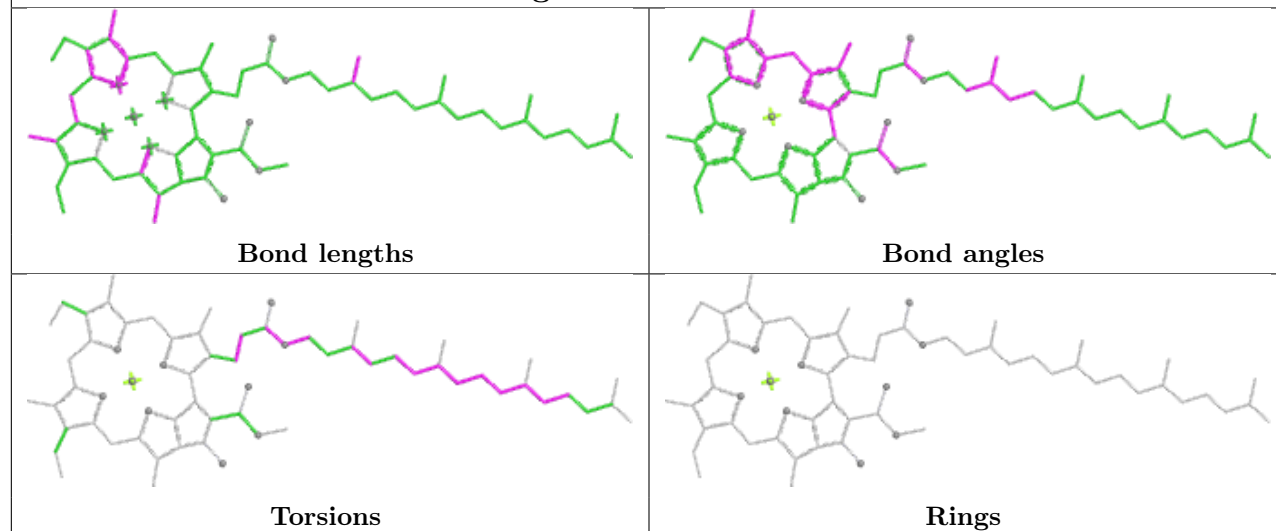
## Ligand CLA A 814



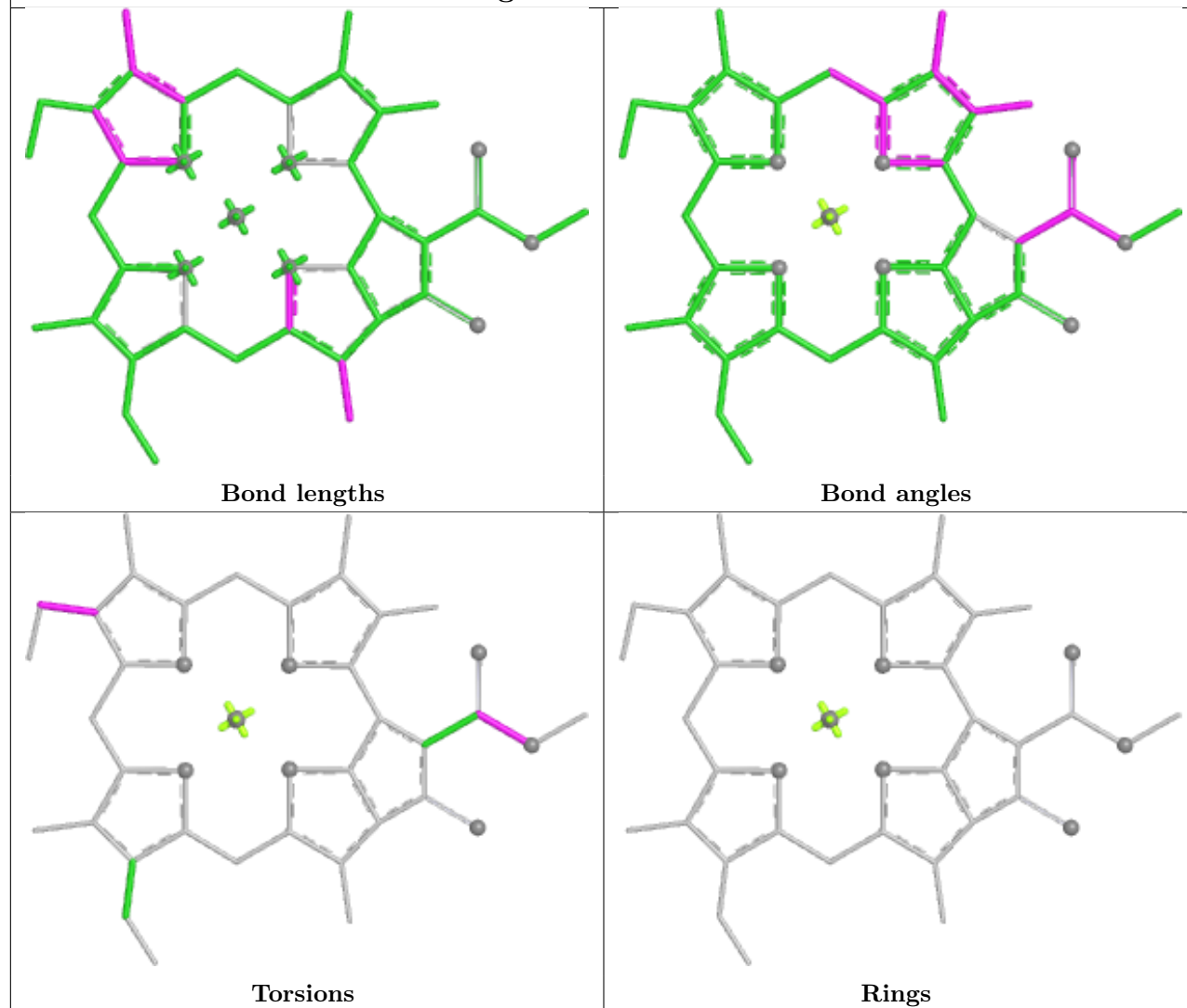
## Ligand LMG b 620

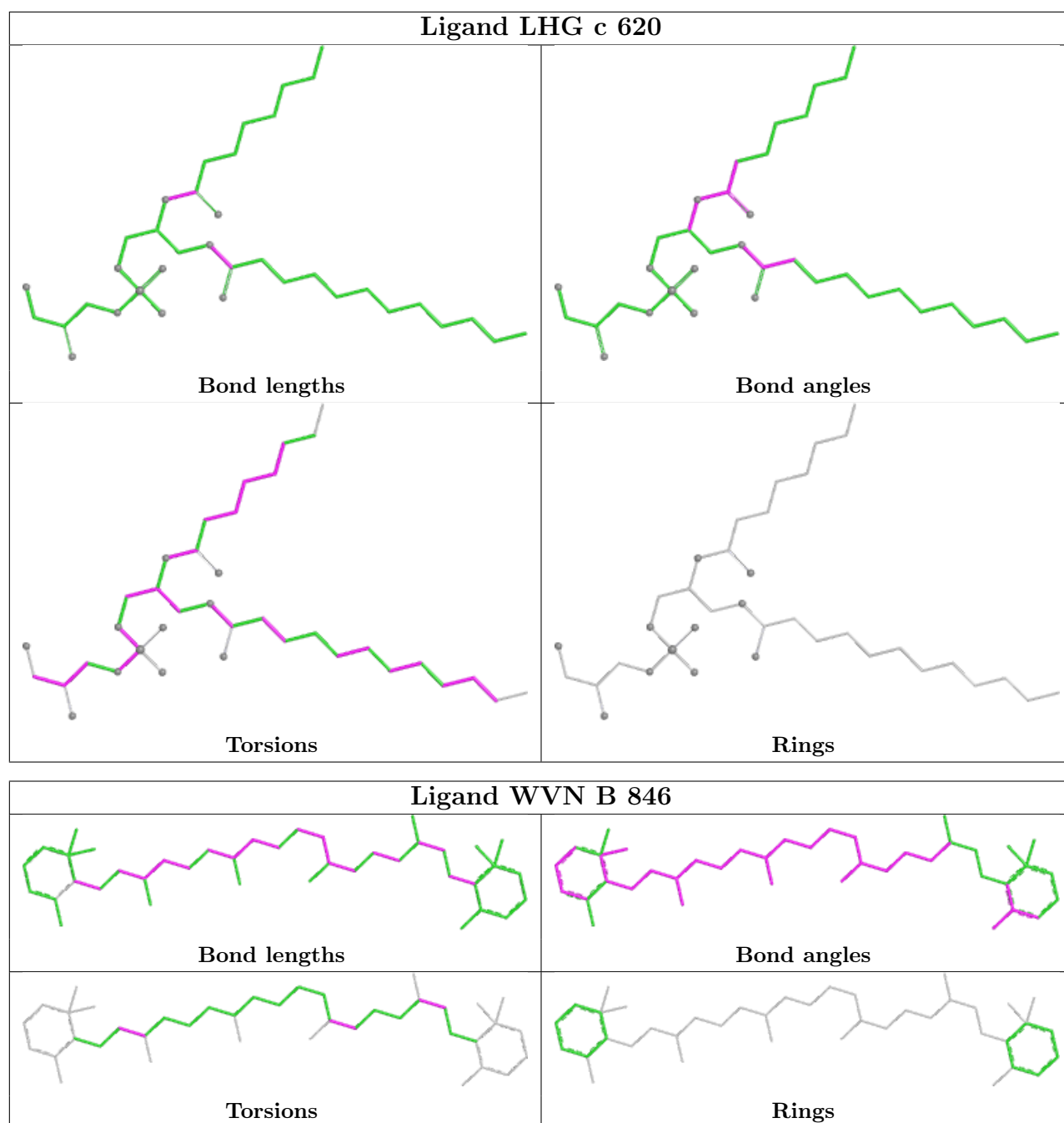


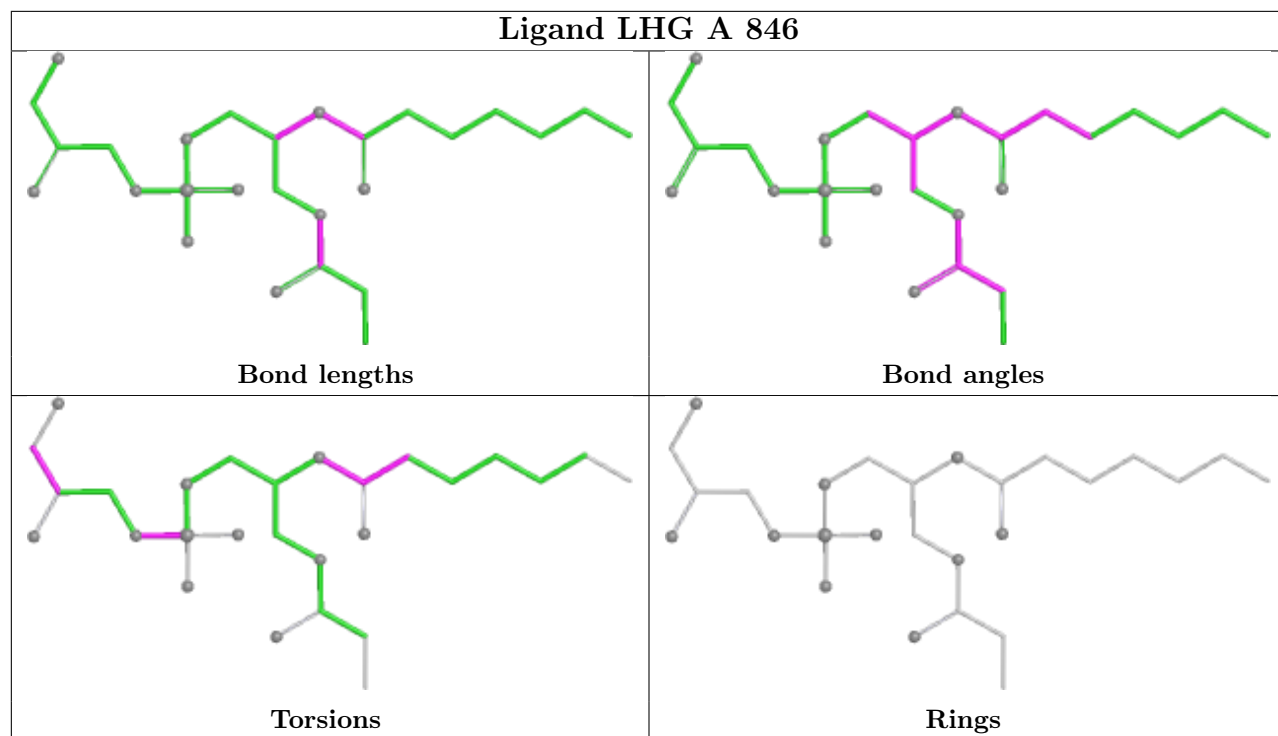
## Ligand CLA B 822



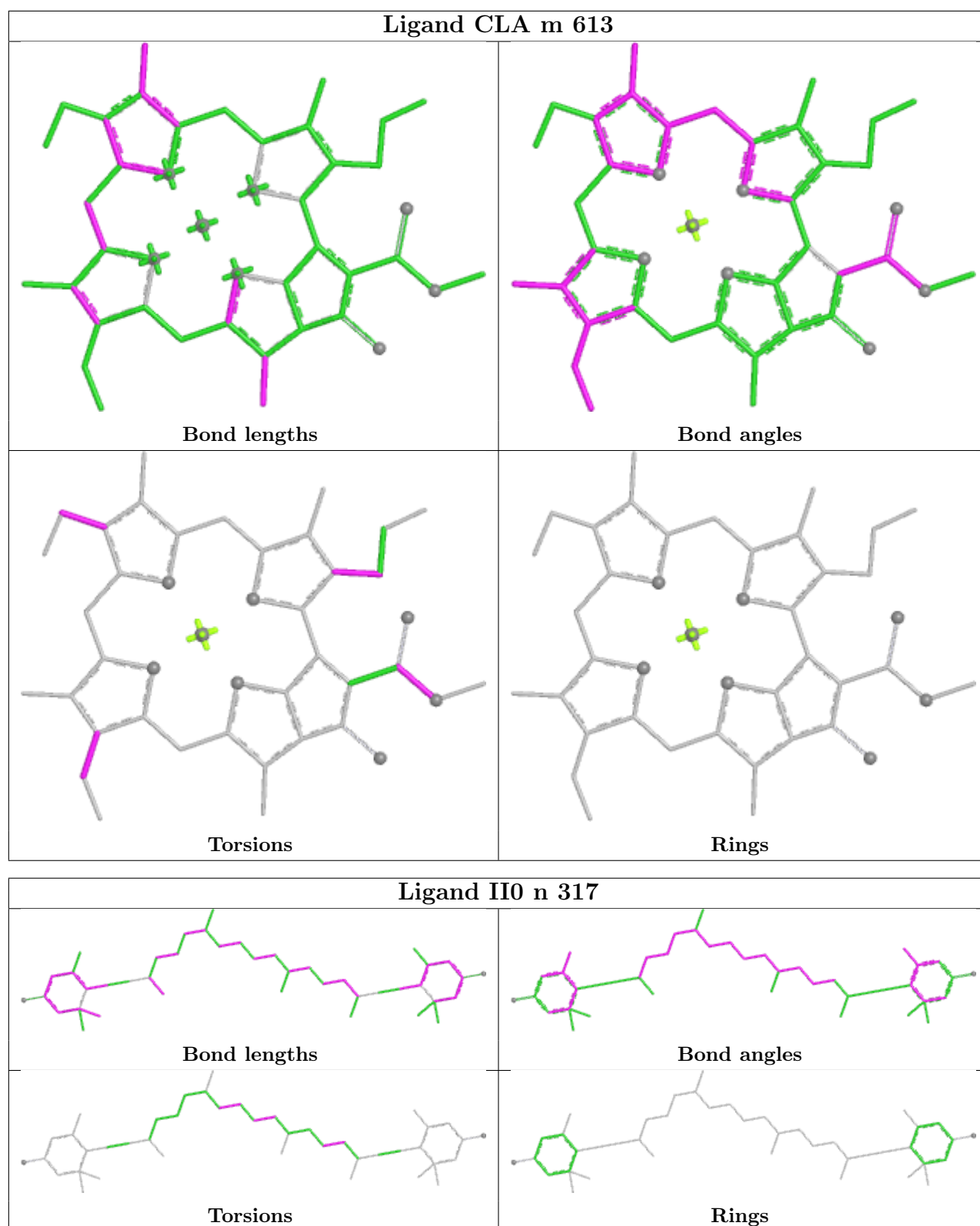
## Ligand CLA d 309

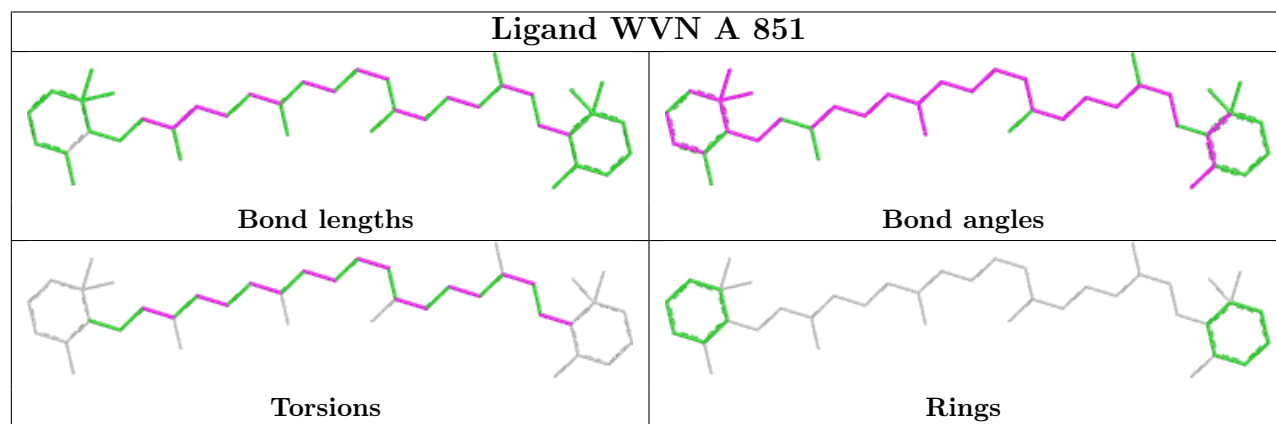
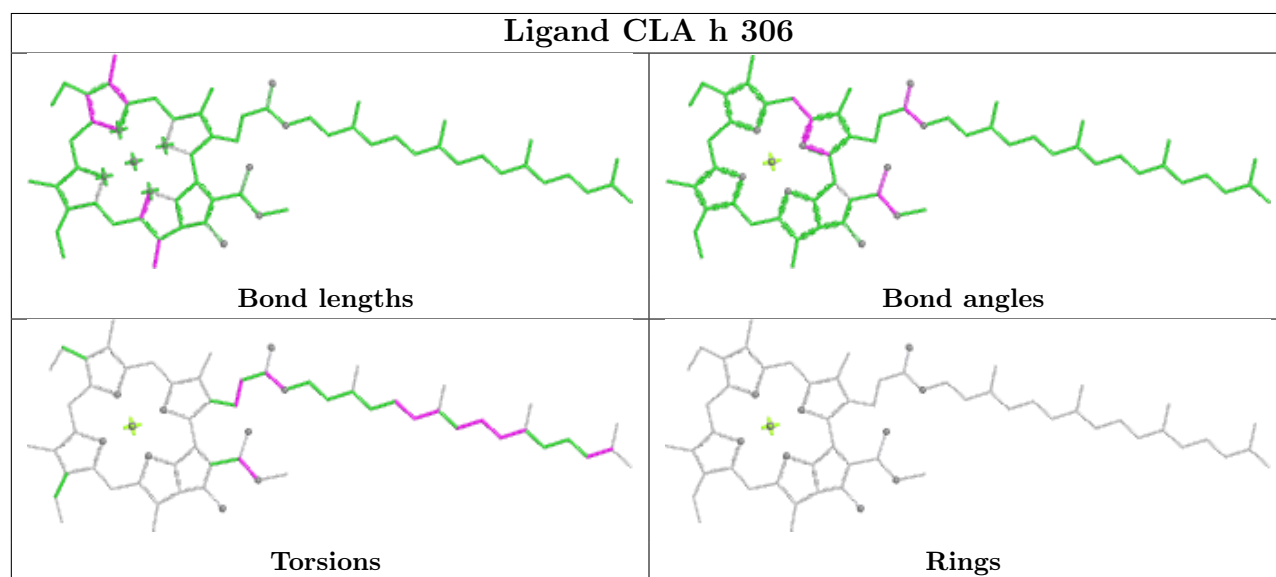
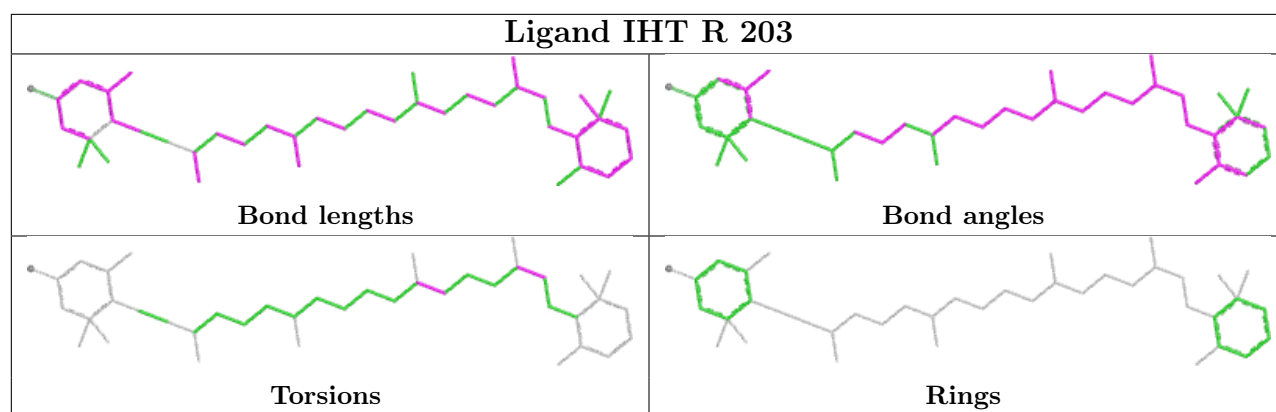


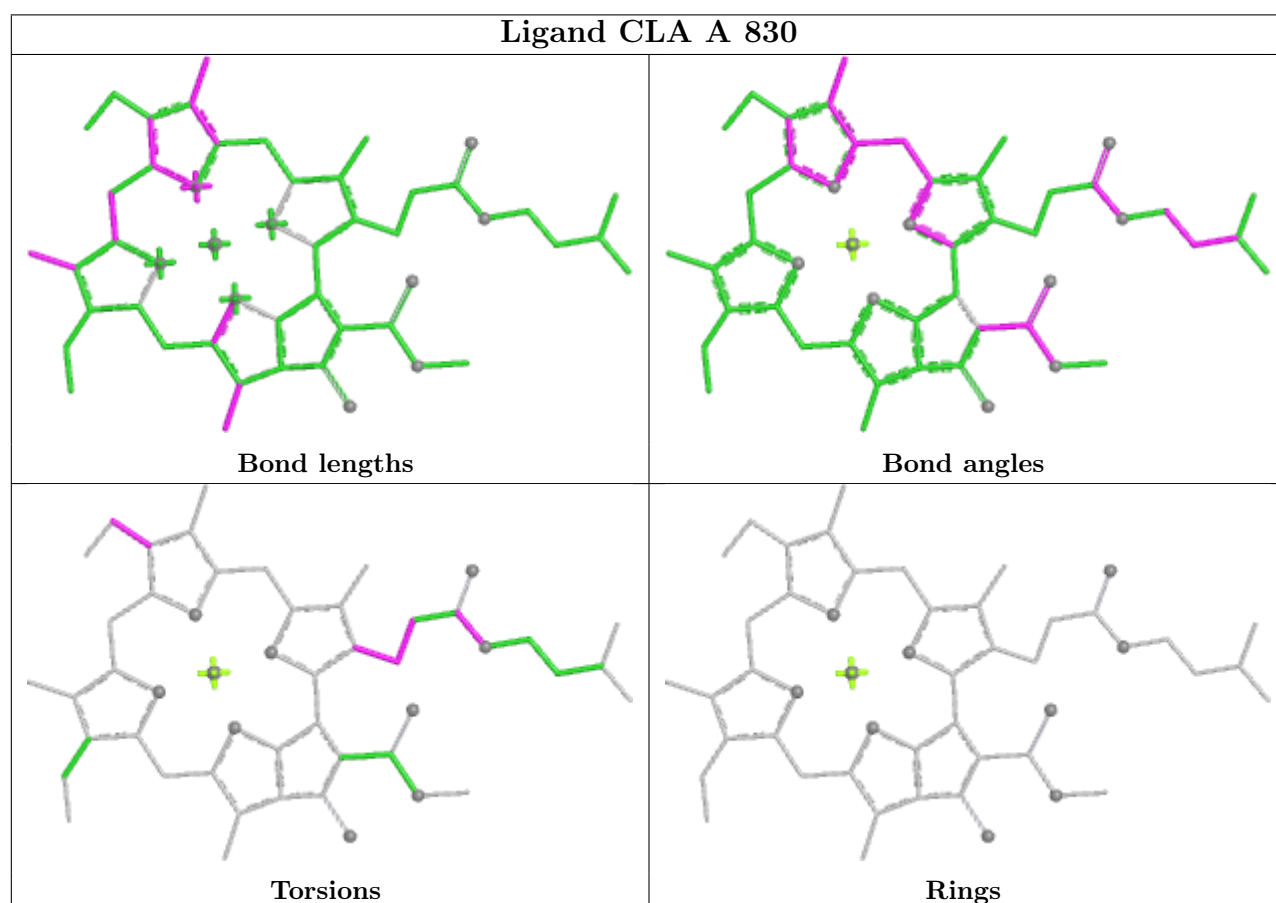
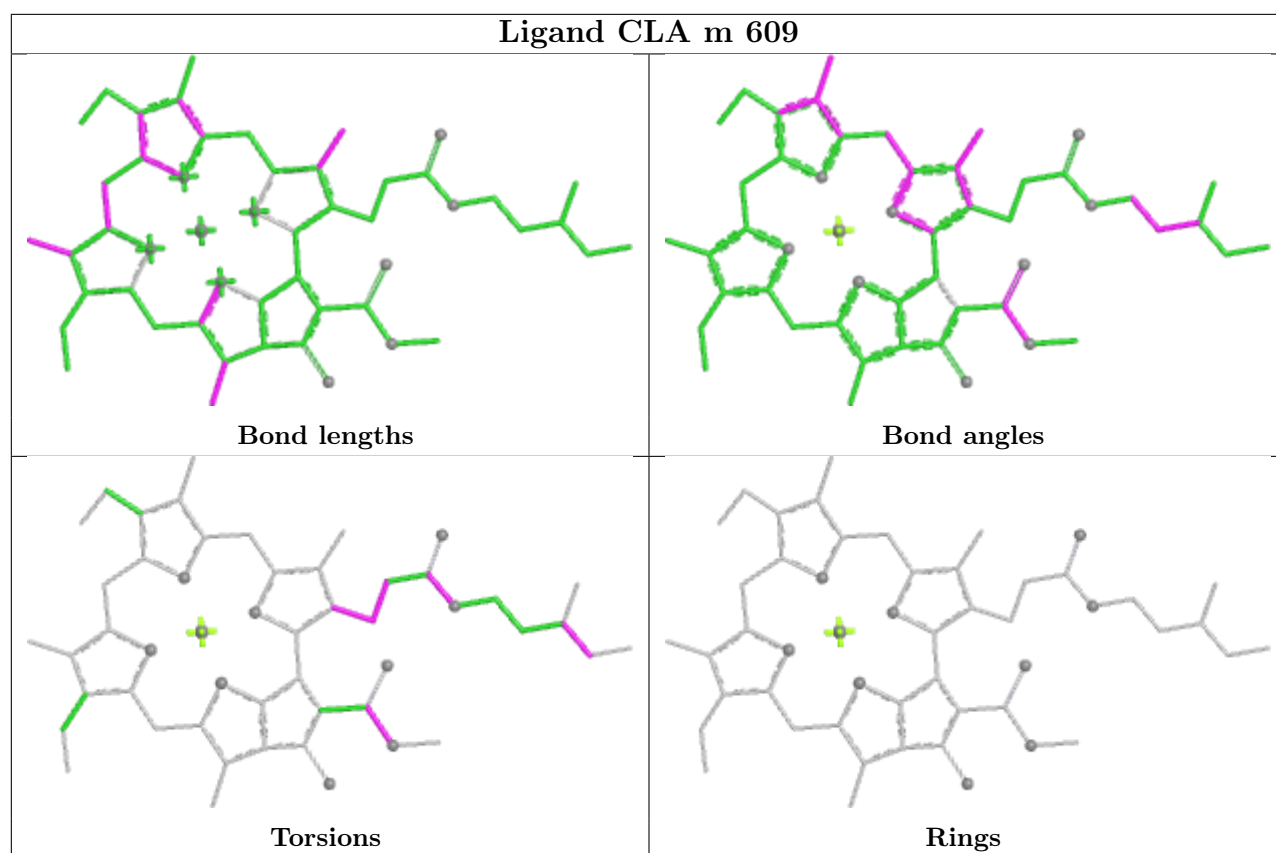


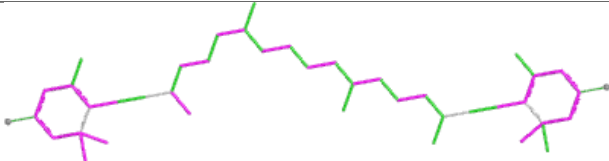
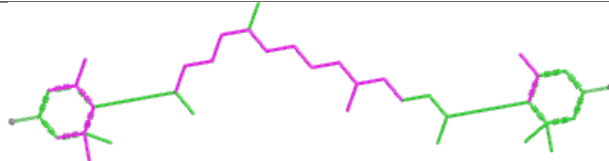
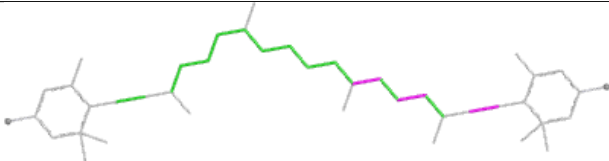
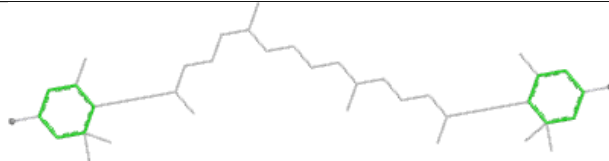


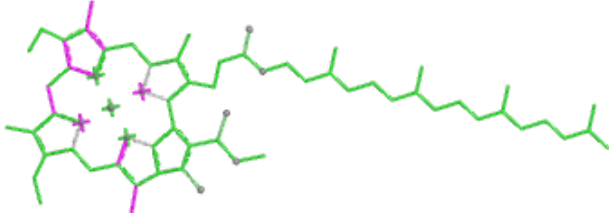
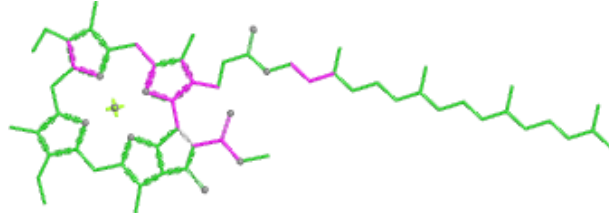
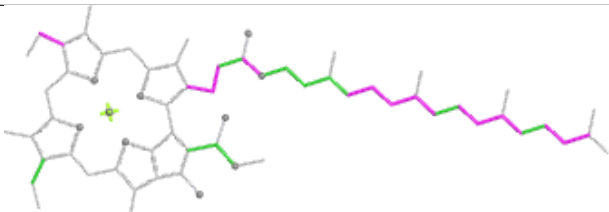
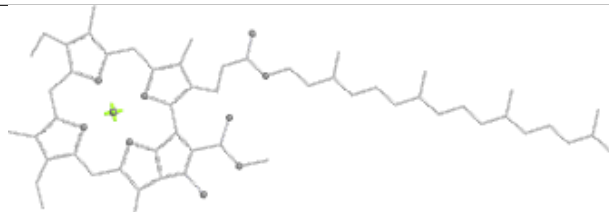


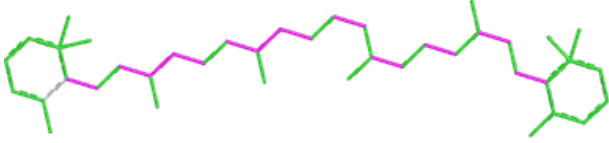
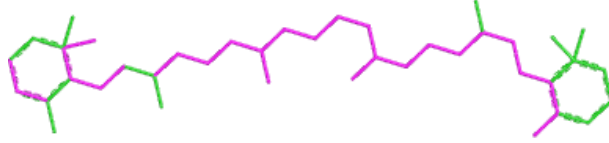
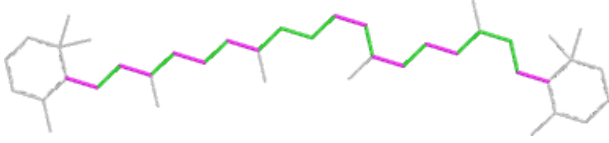
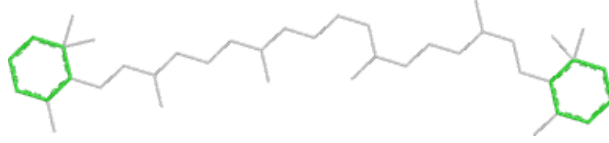


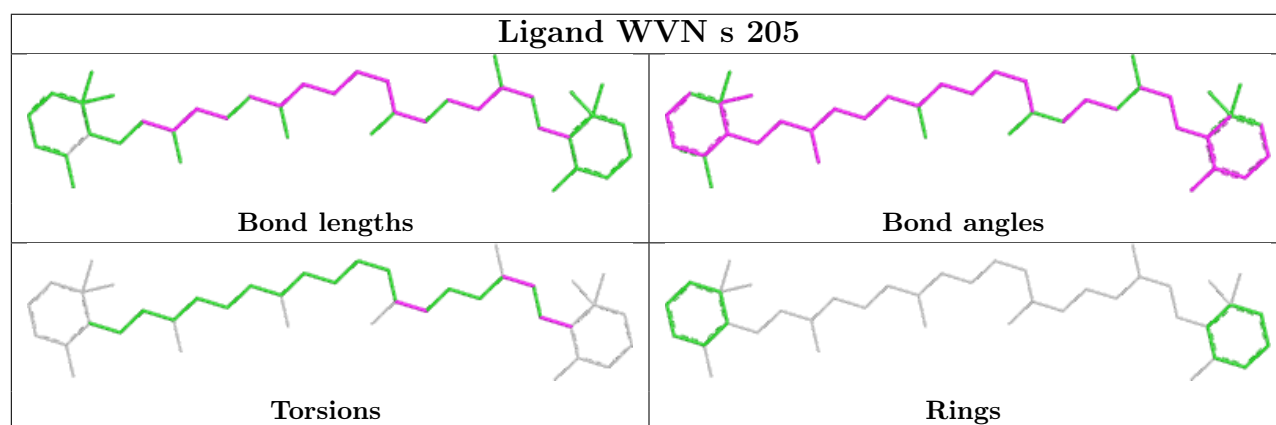
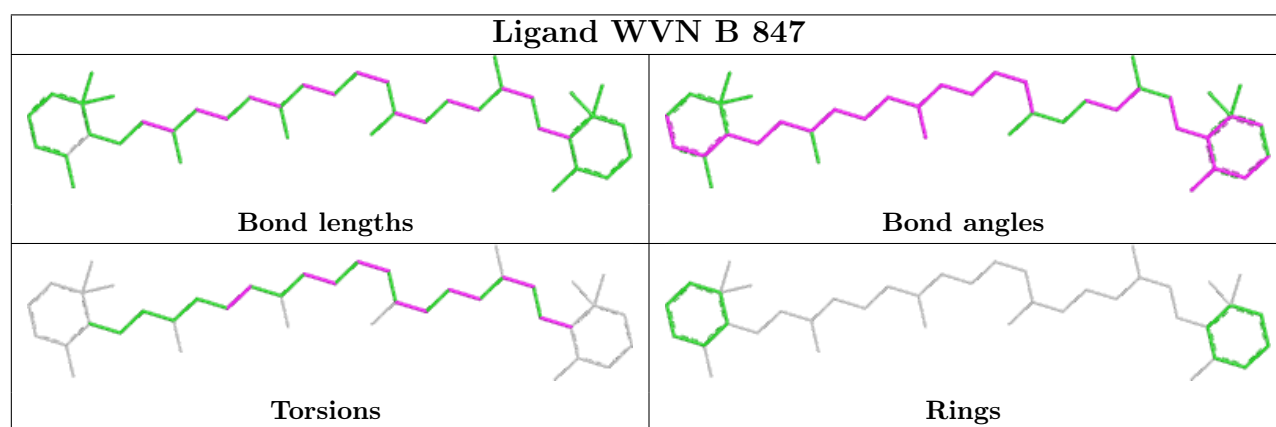
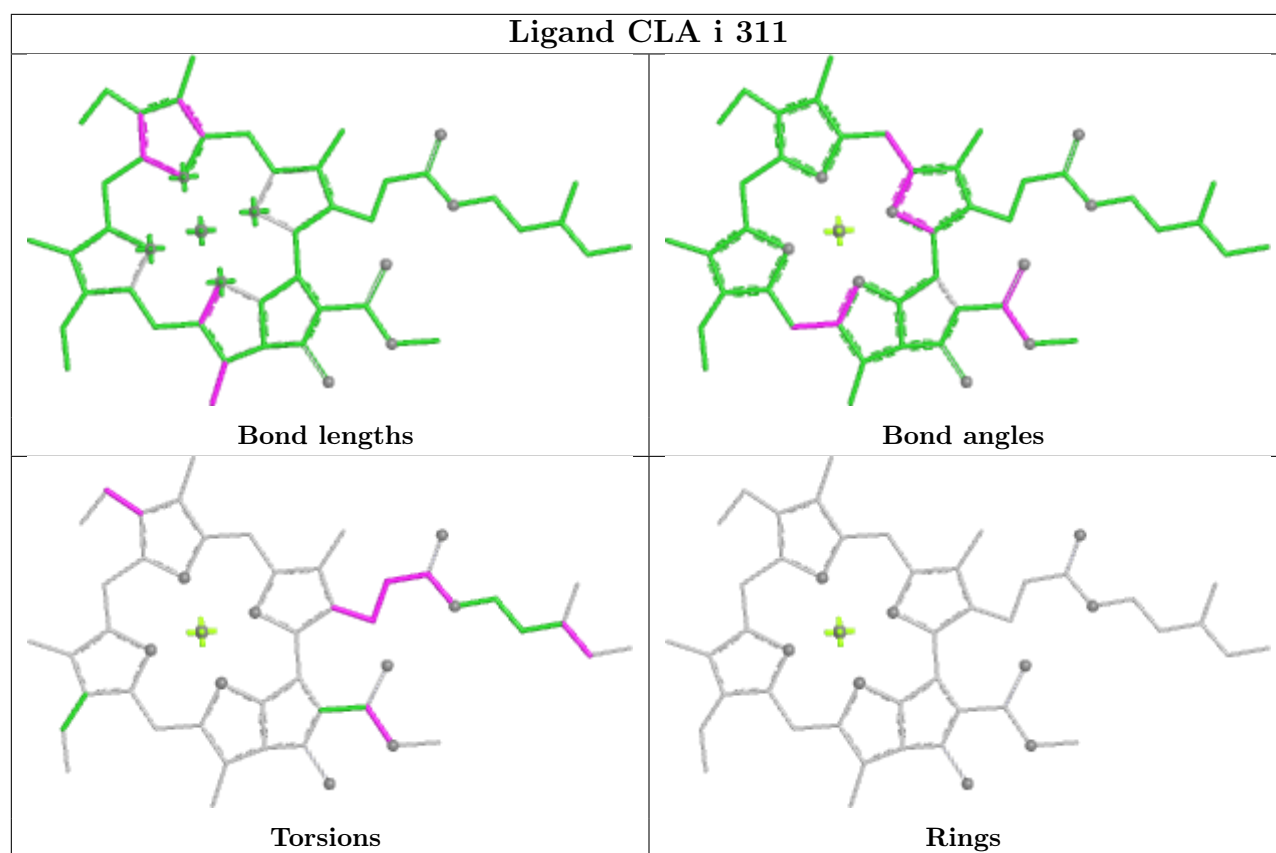




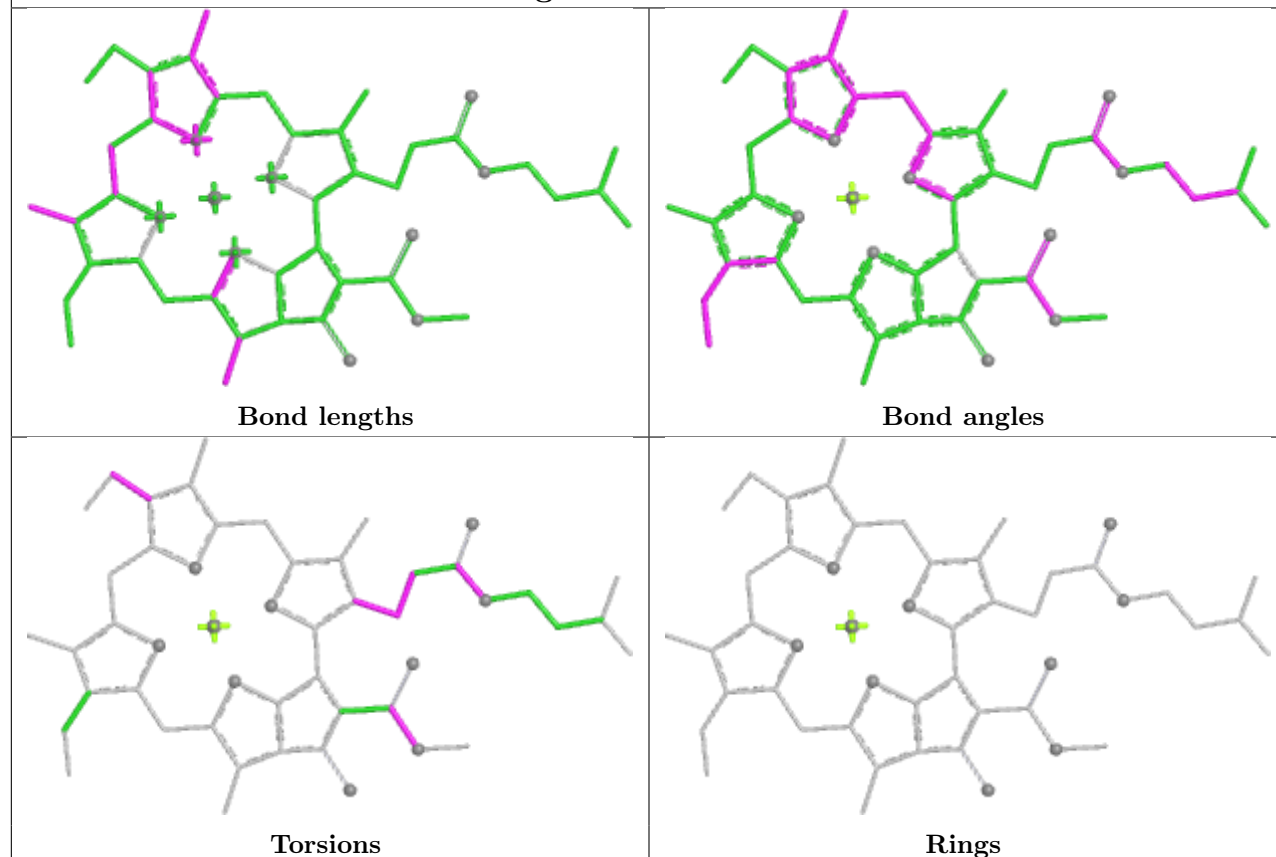
| Ligand II0 c 613                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand CLA a 312                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

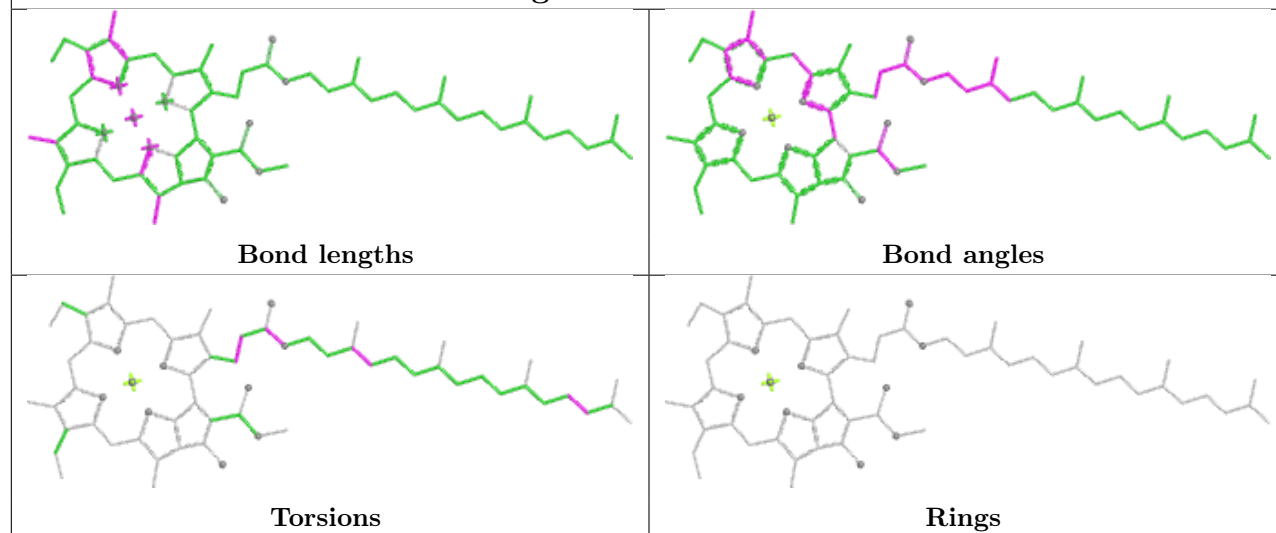
| Ligand WVN F 204                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



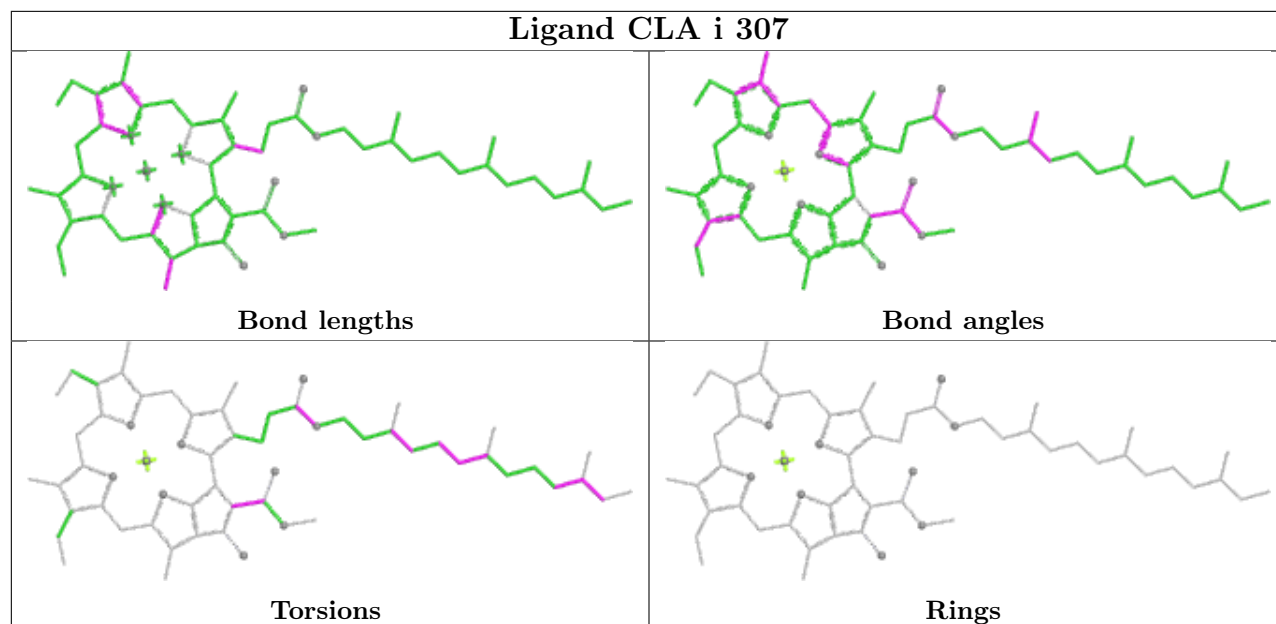
## Ligand CLA h 302



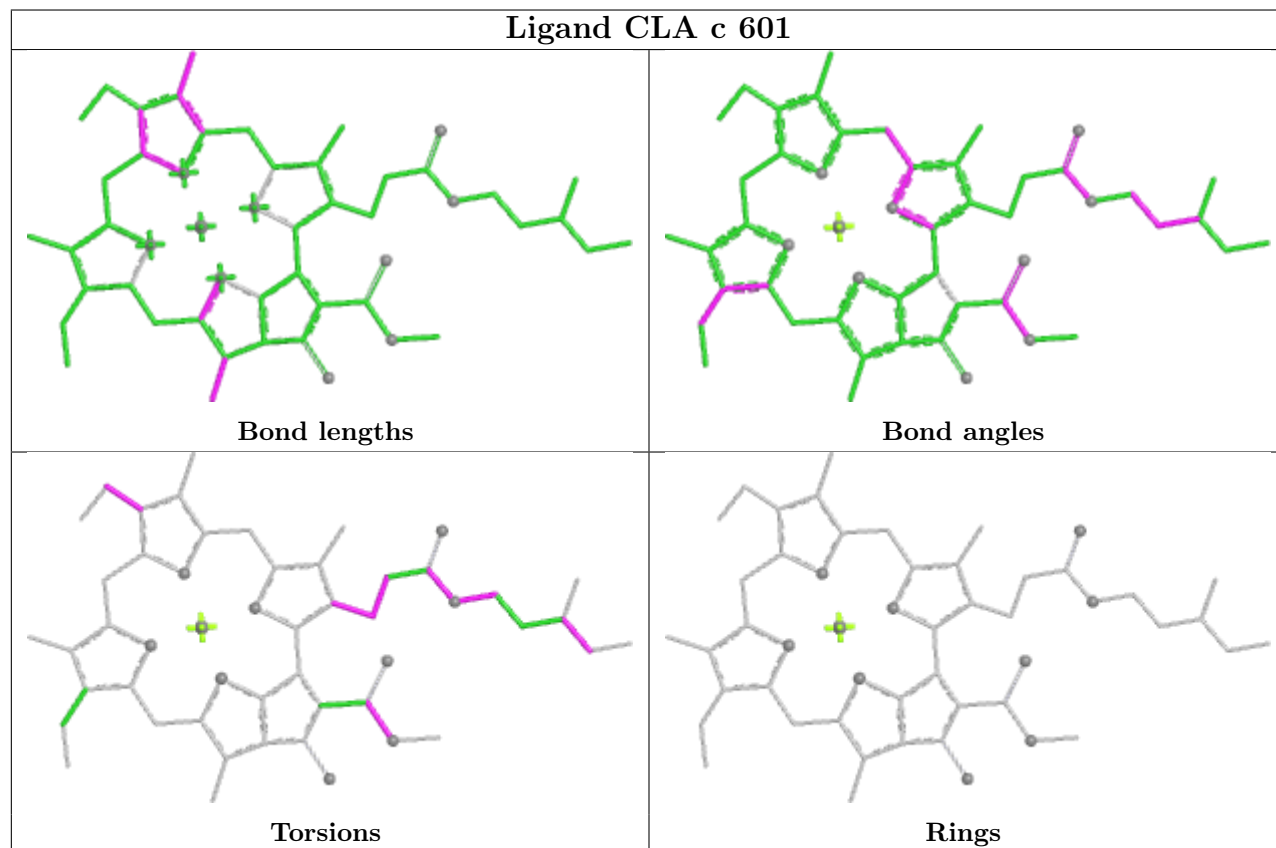
## Ligand CLA A 828



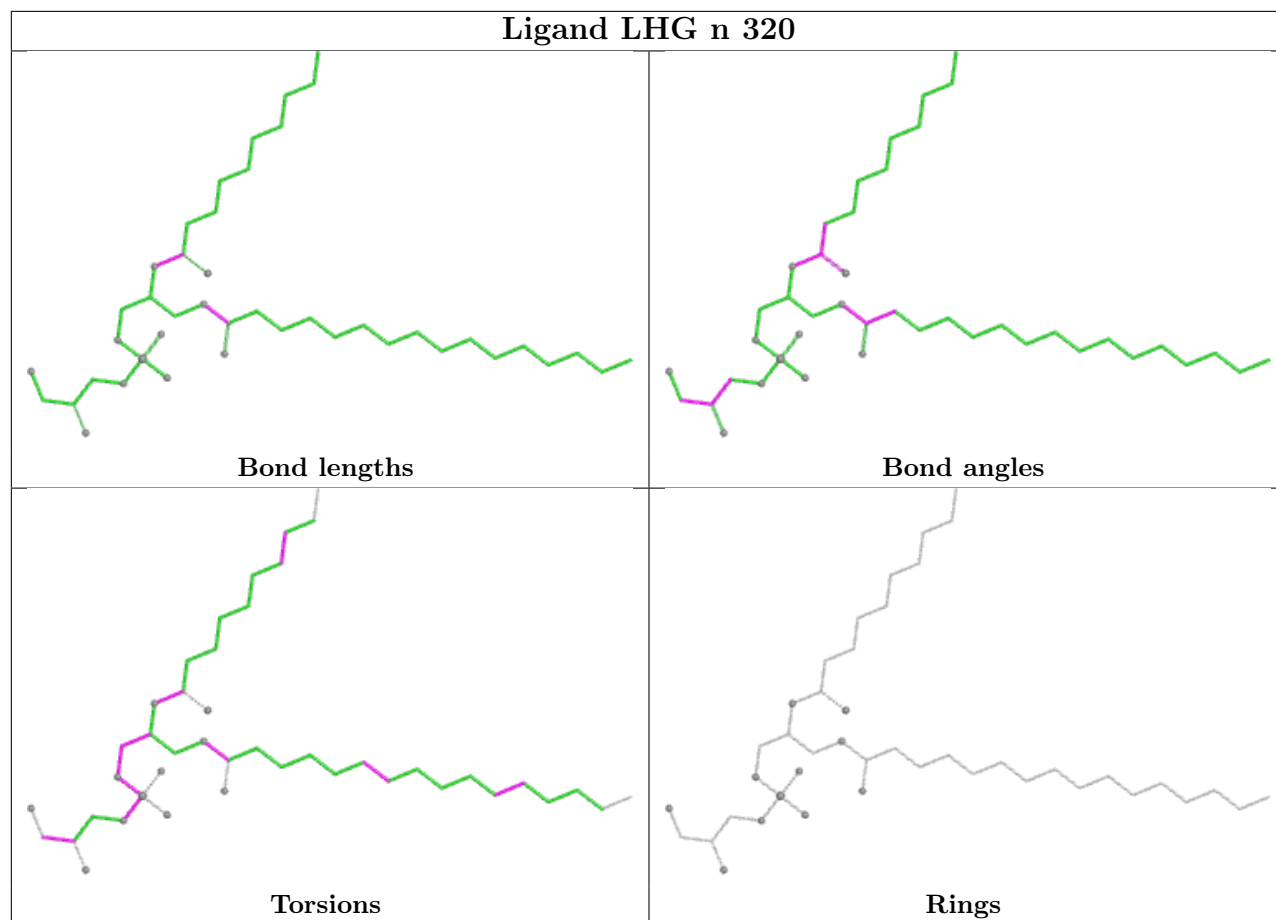
## Ligand CLA i 307



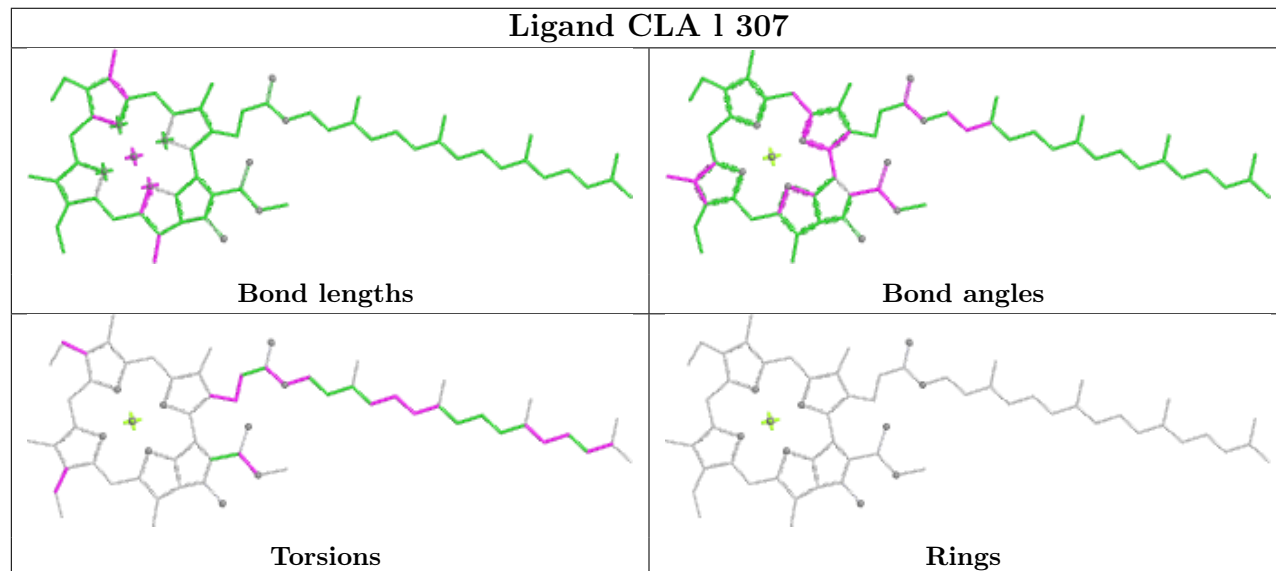
## Ligand CLA c 601



## Ligand LHG n 320

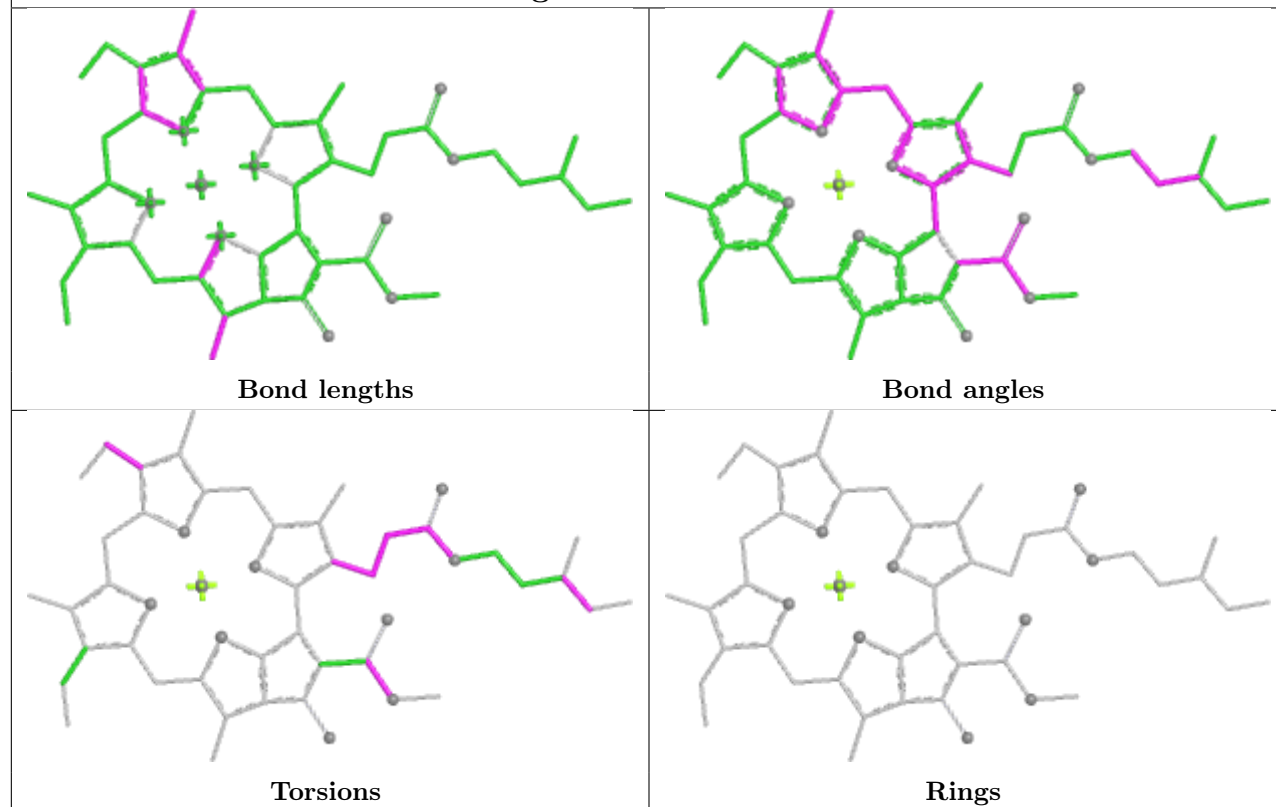


## Ligand CLA 1 307

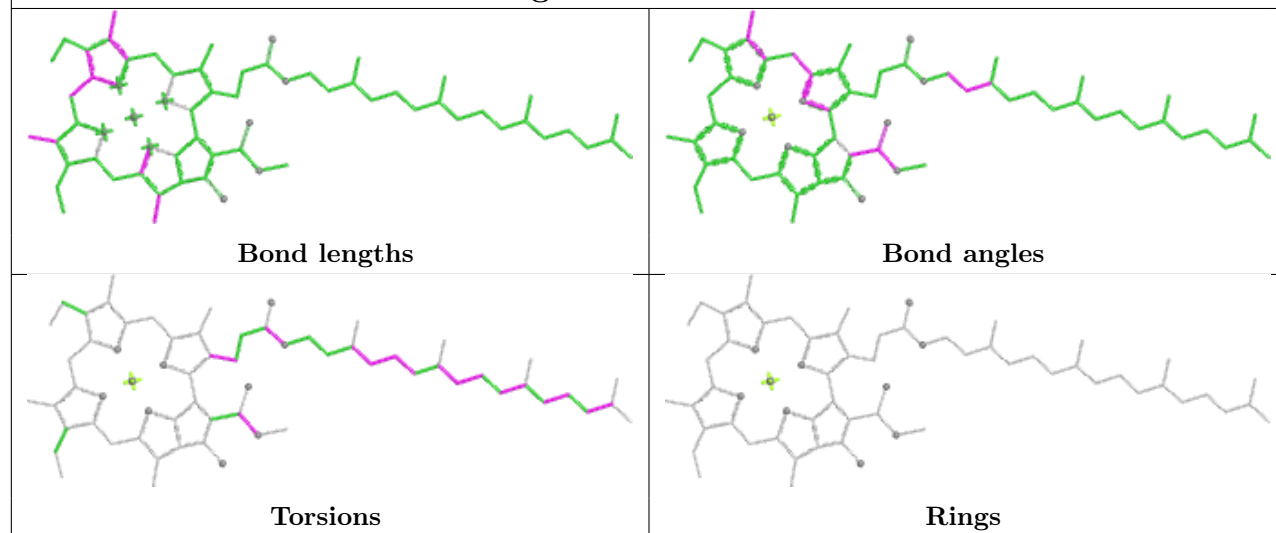




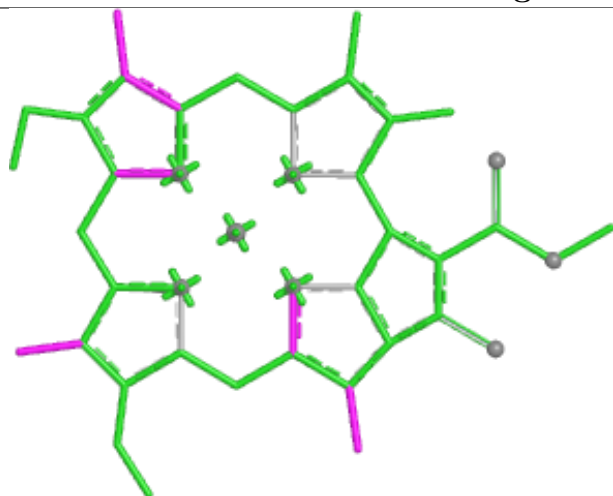
## Ligand CLA R 202



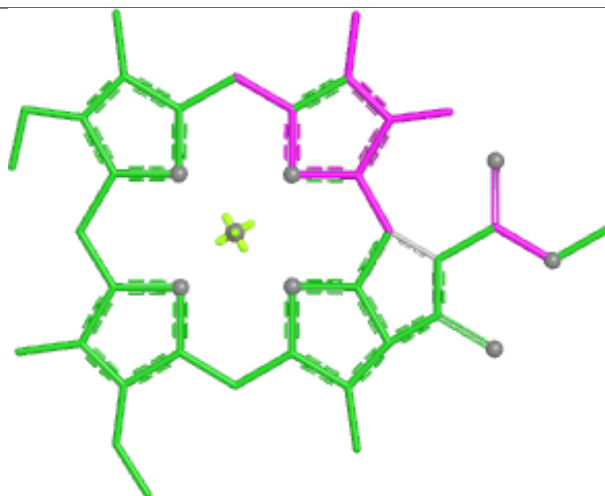
## Ligand CLA A 829



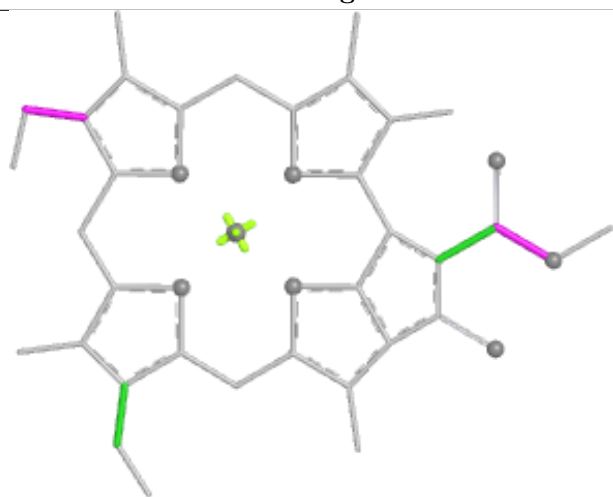
## Ligand CLA A 856



Bond lengths



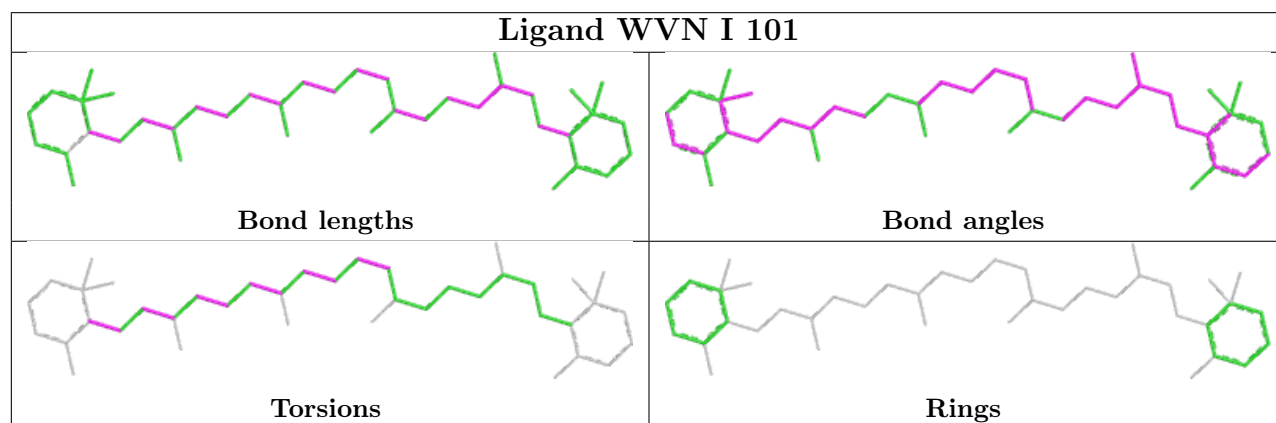
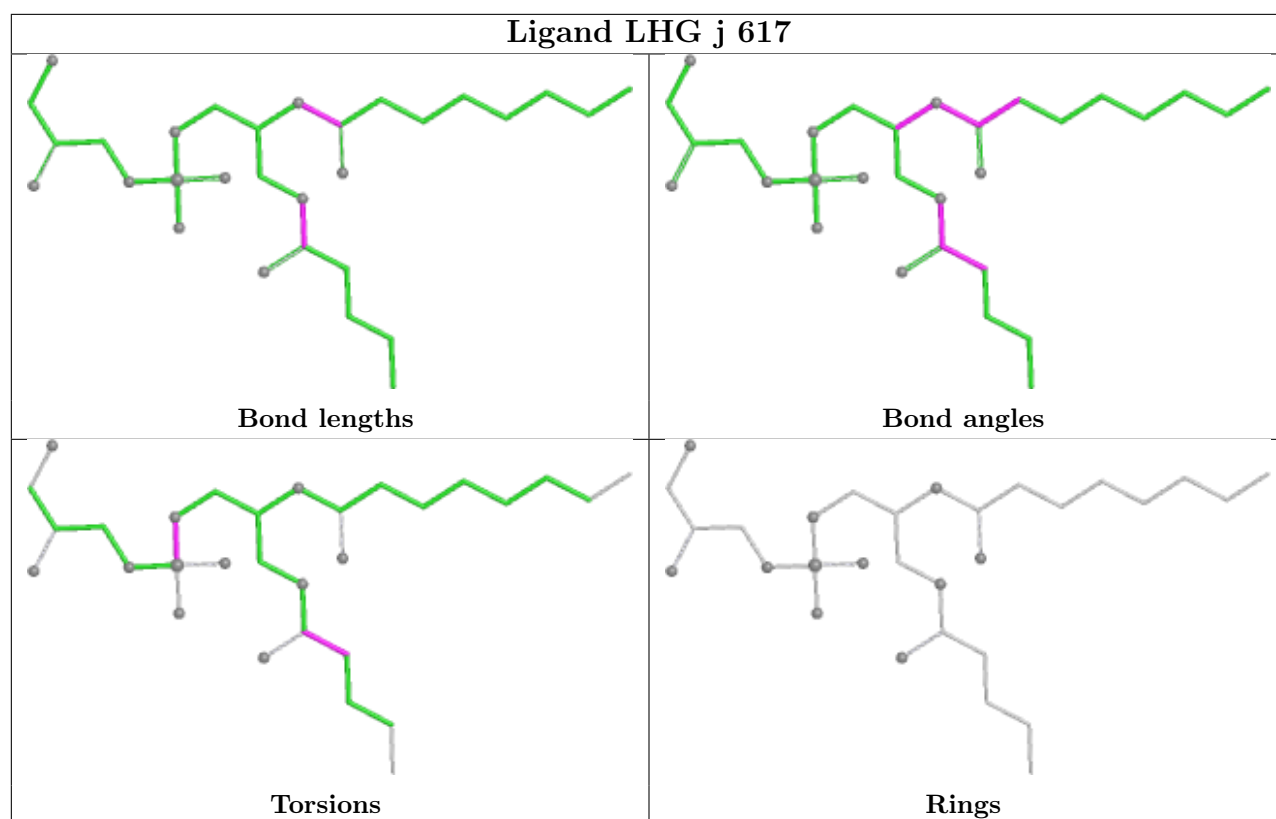
Bond angles

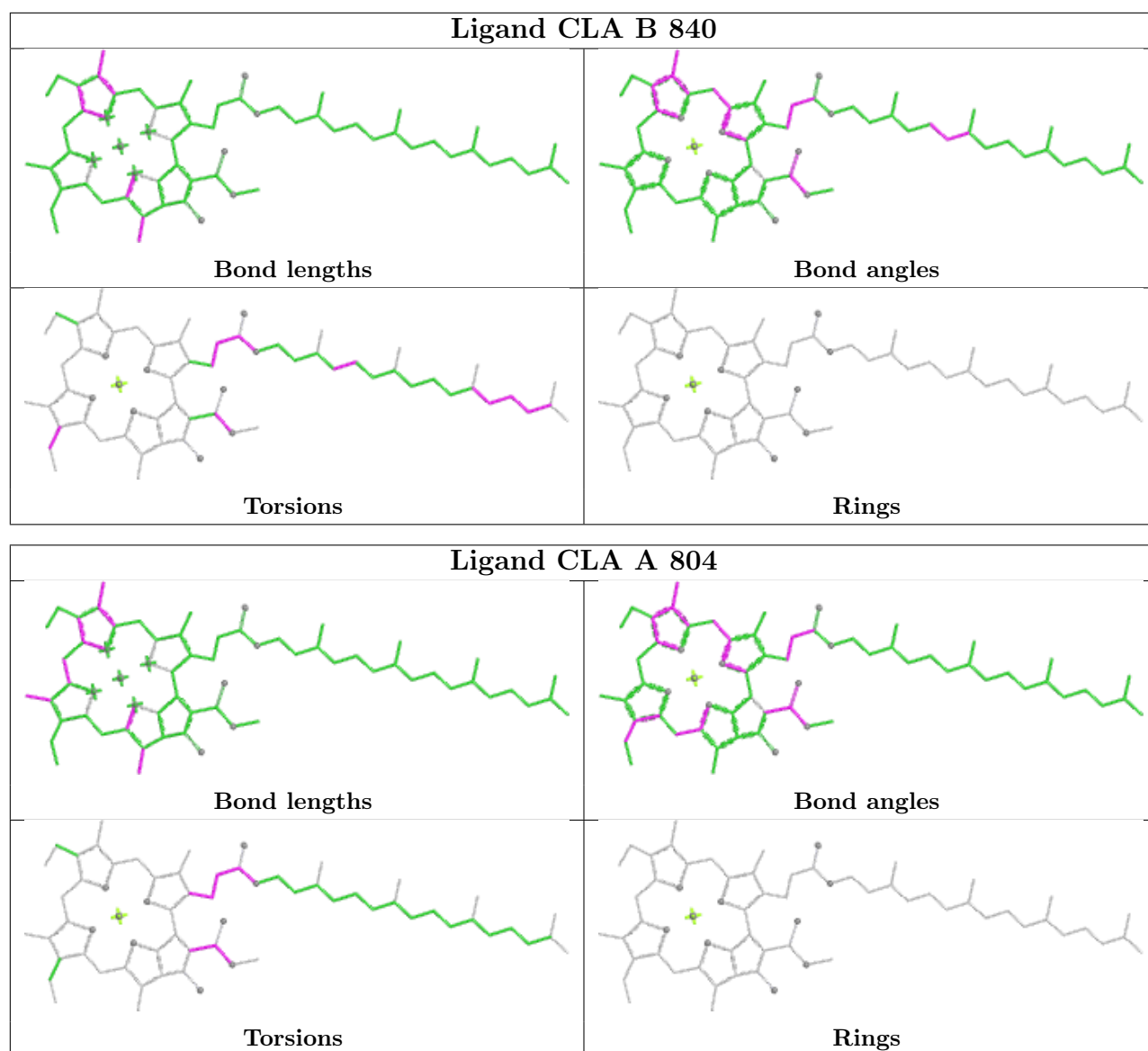


Torsions

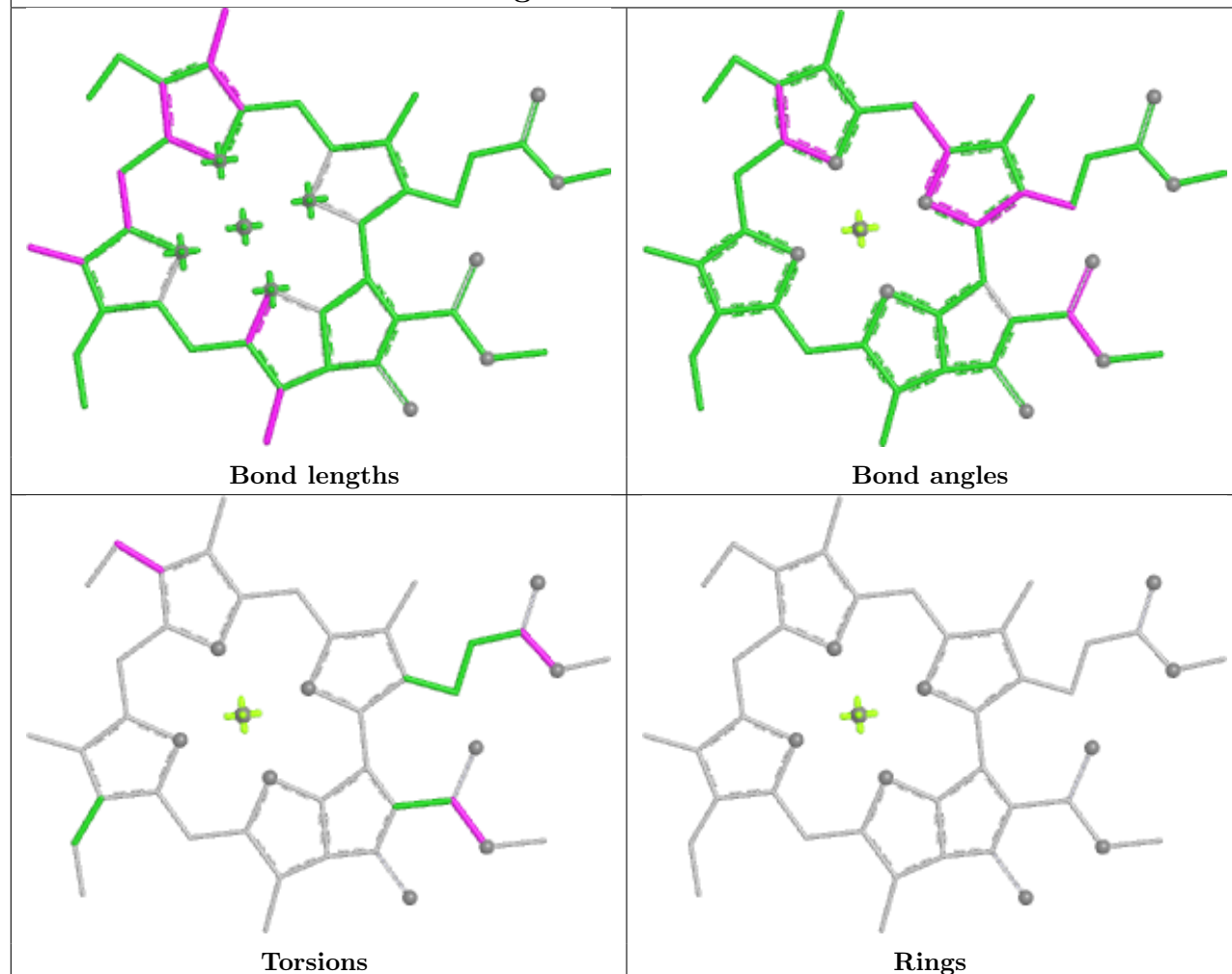


Rings





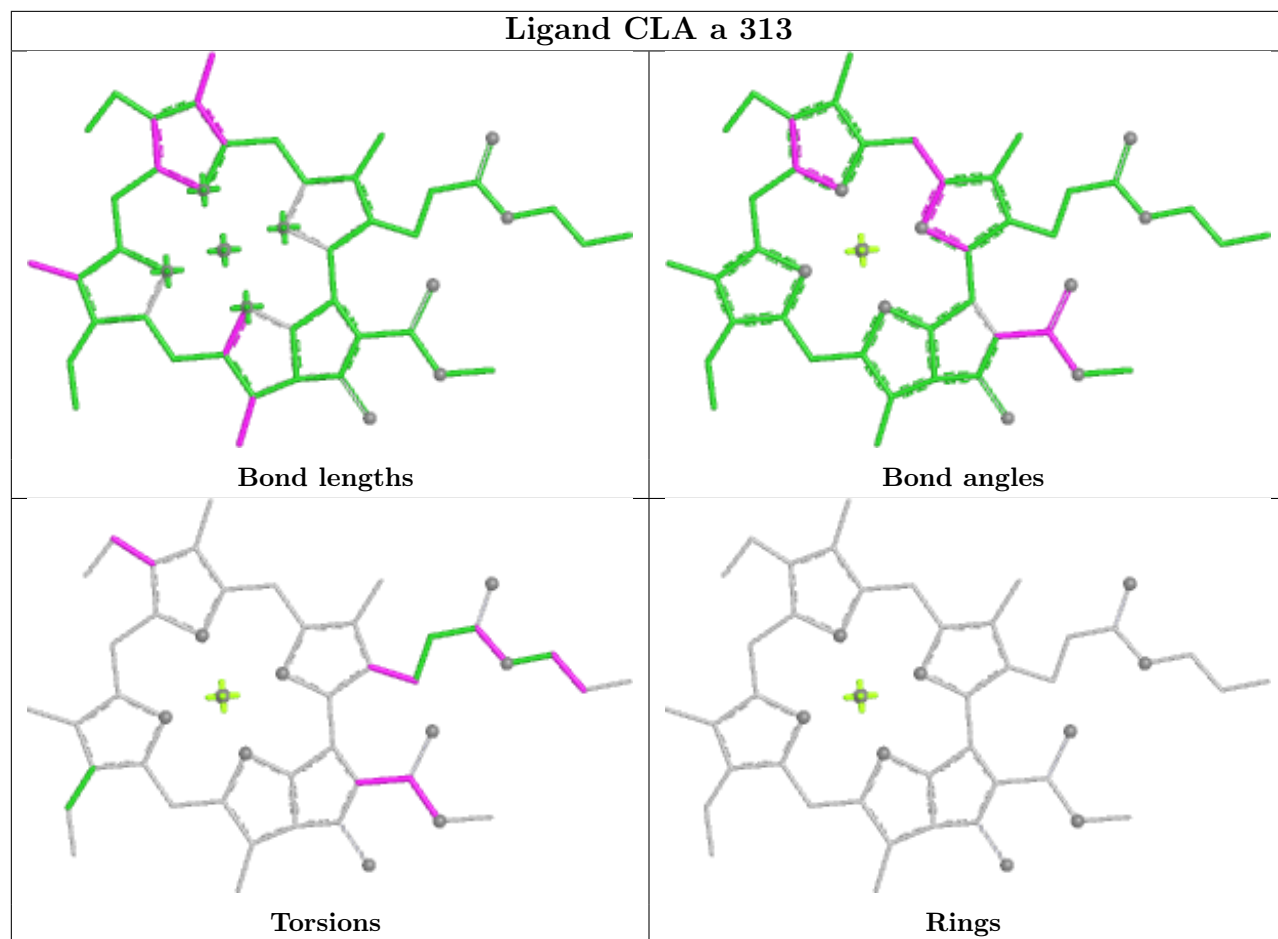
## Ligand CLA B 819

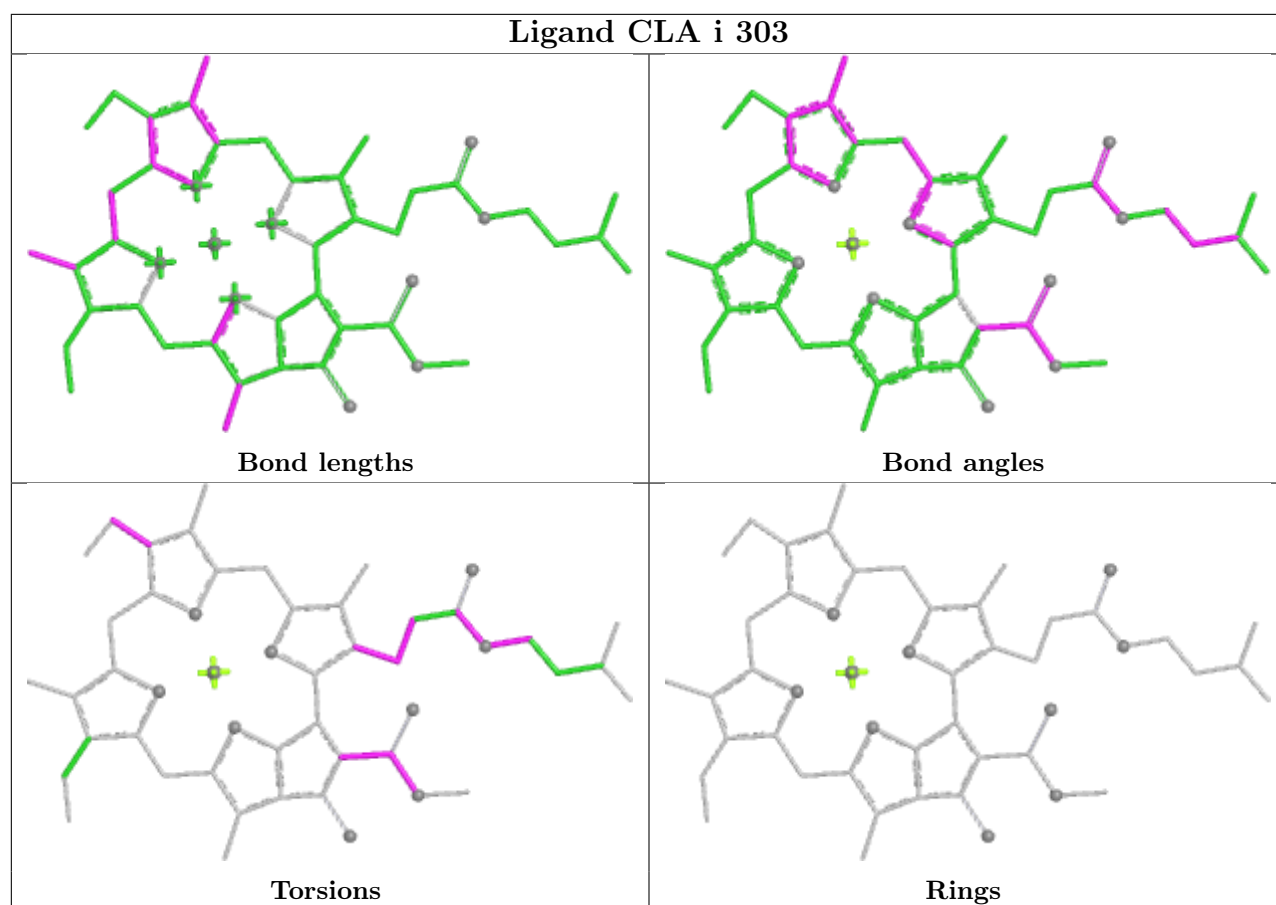


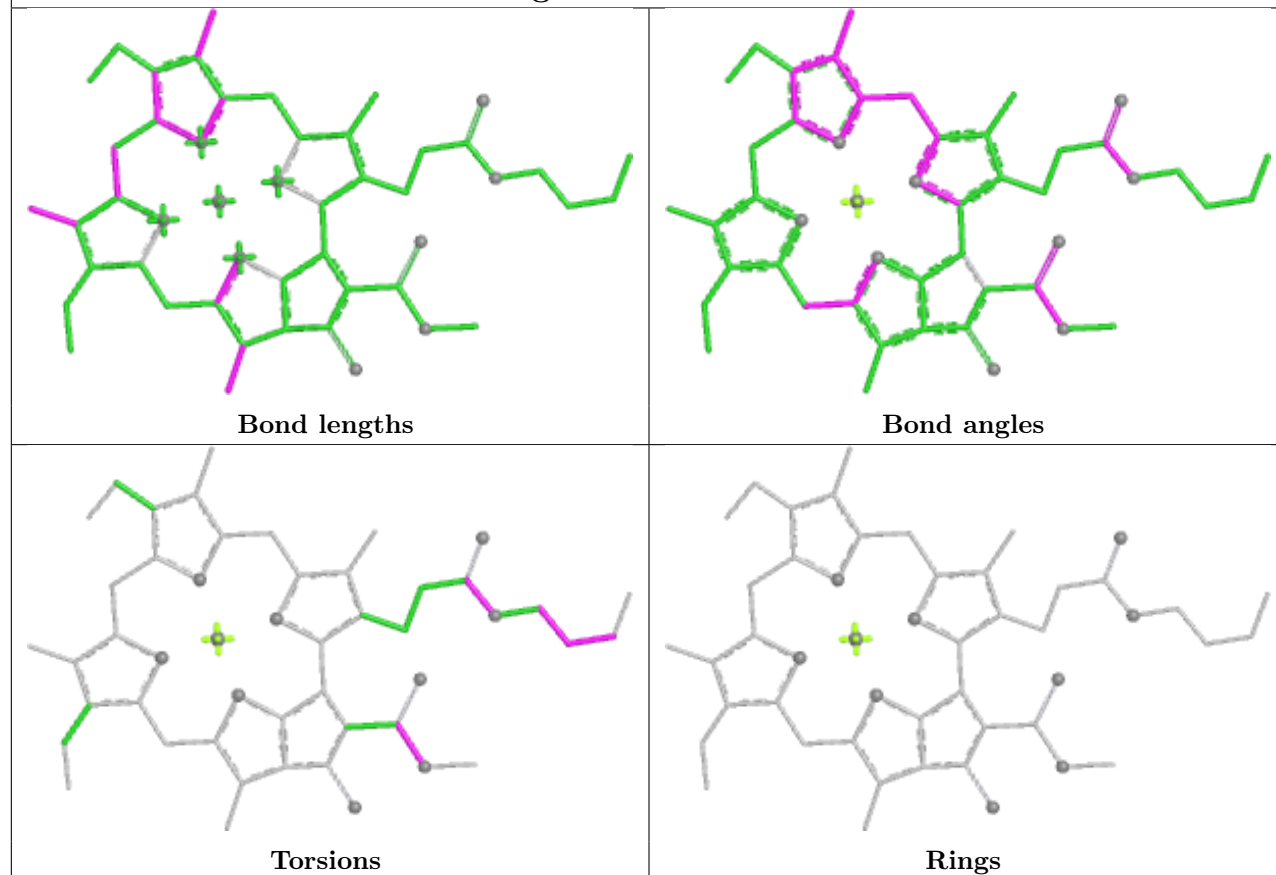
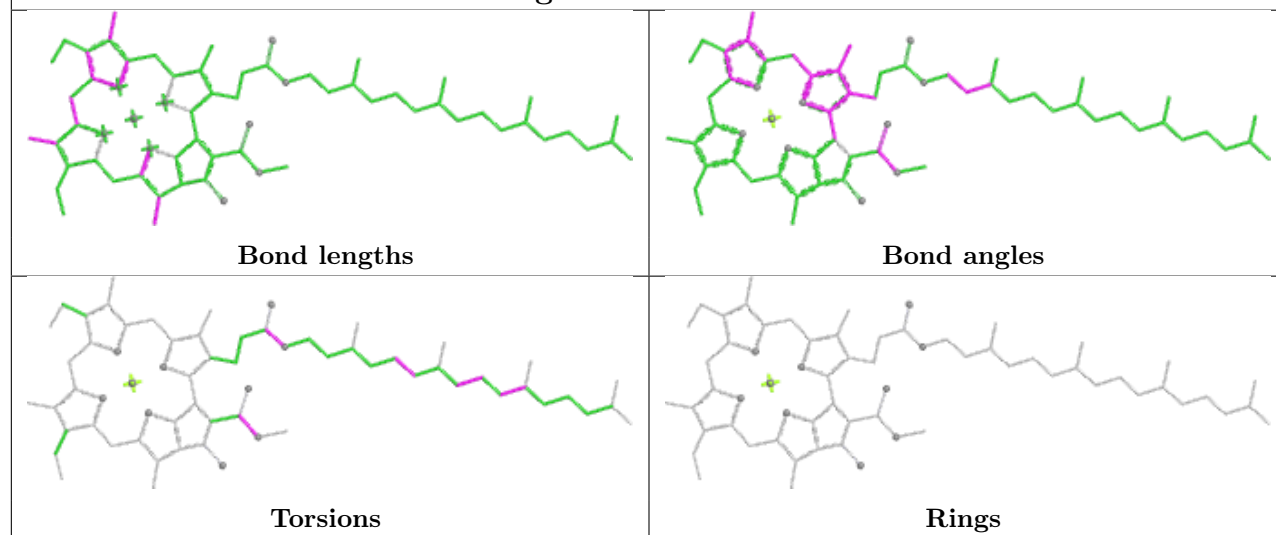
## Ligand LMG s 208



## Ligand CLA a 313

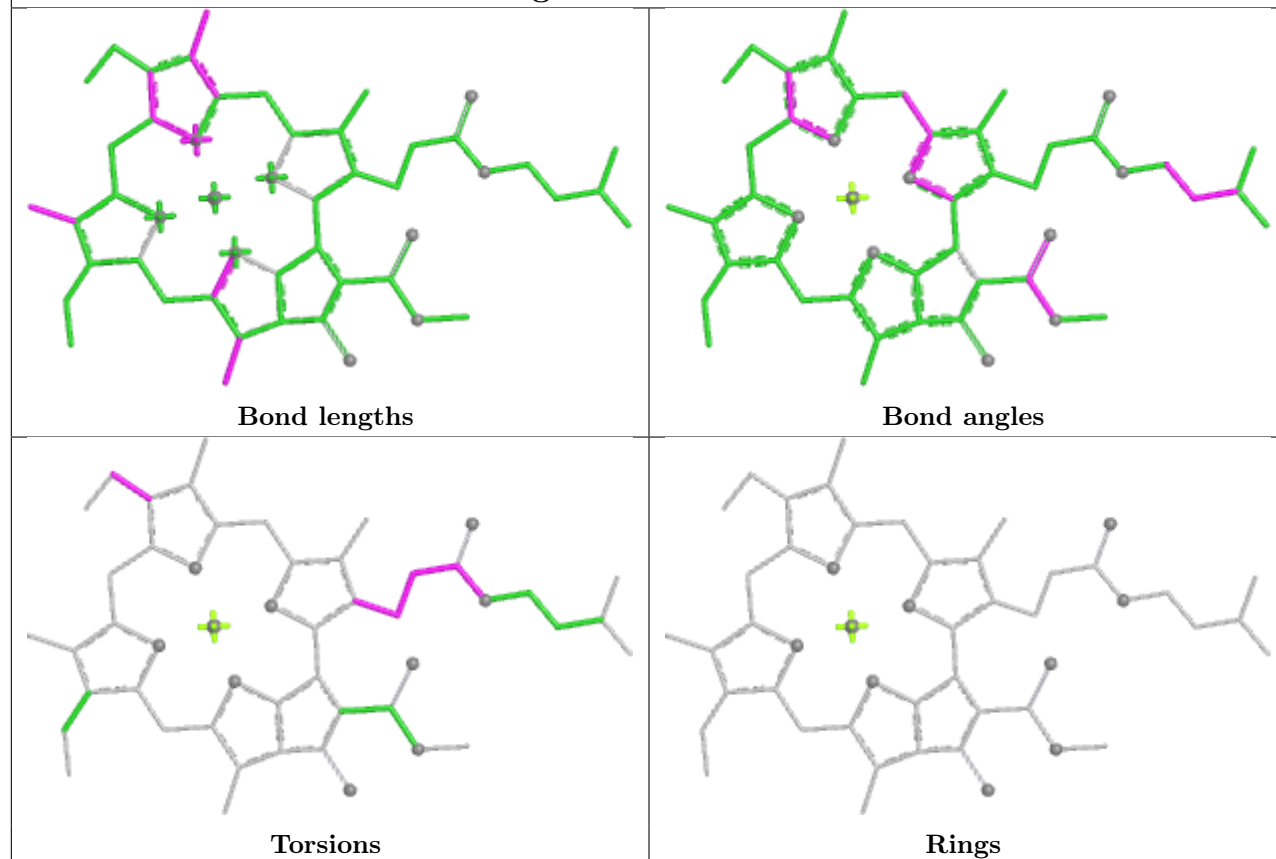




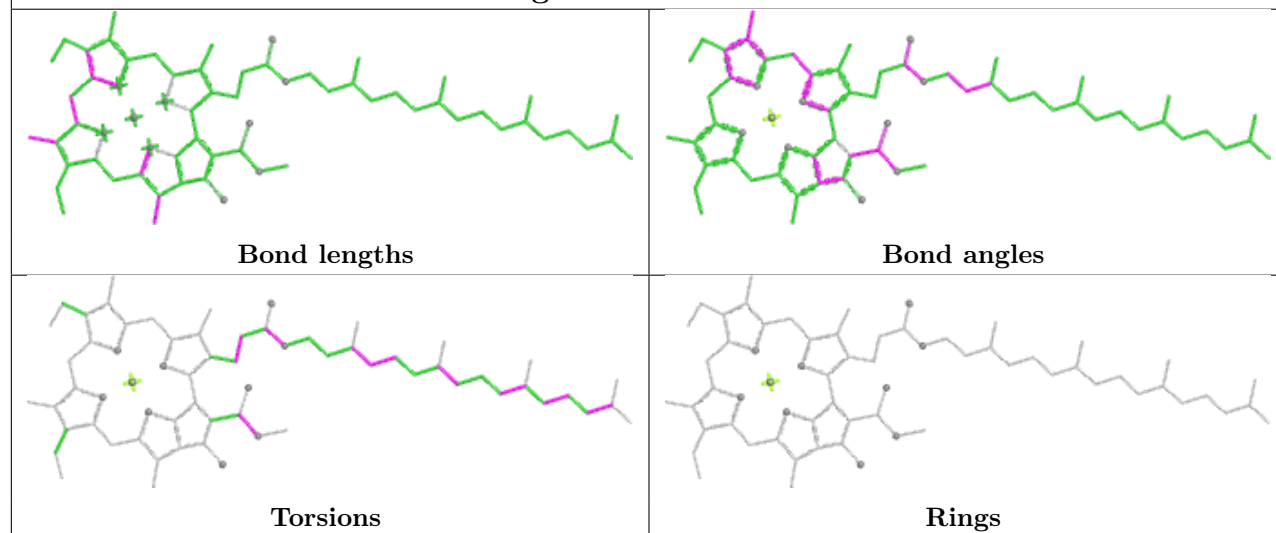
**Ligand CLA B 828****Ligand CLA b 603**

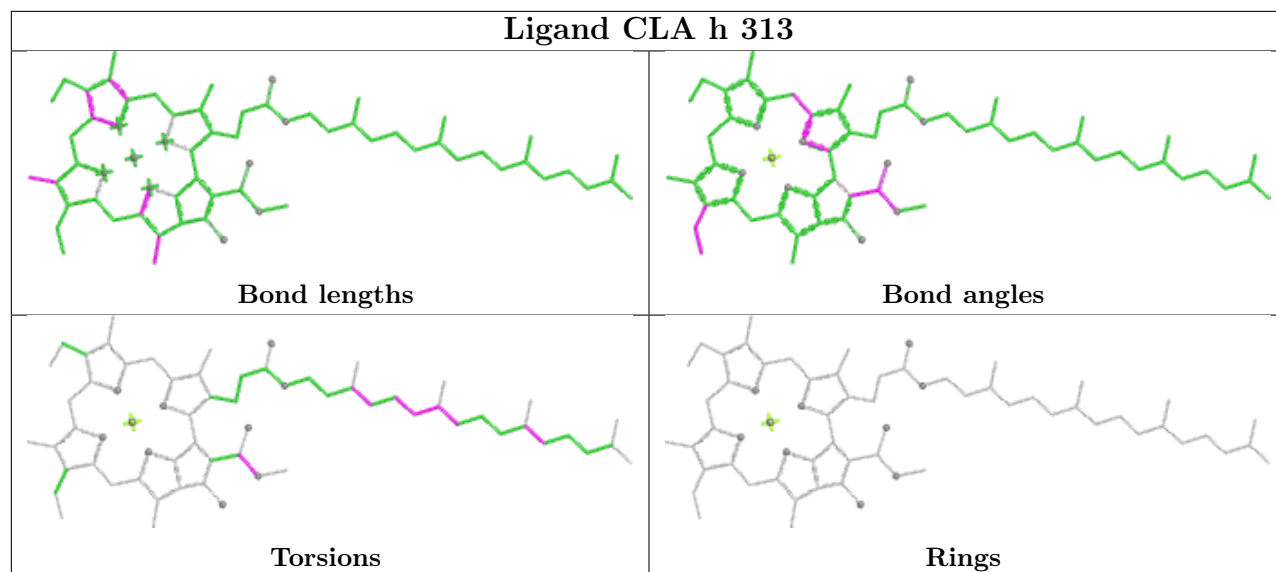
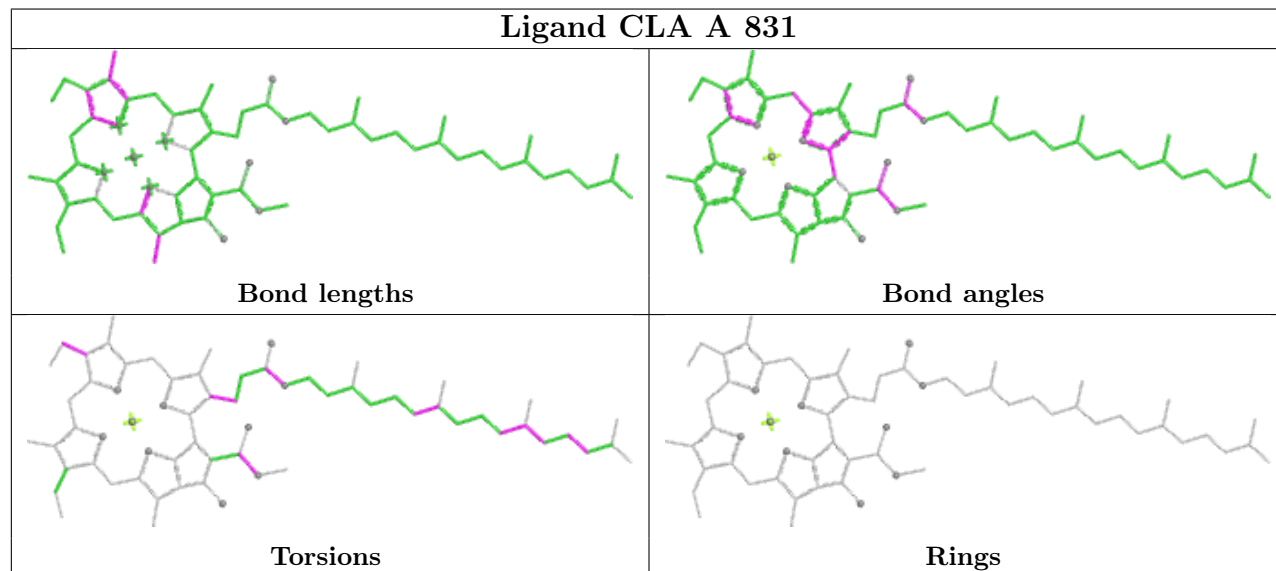


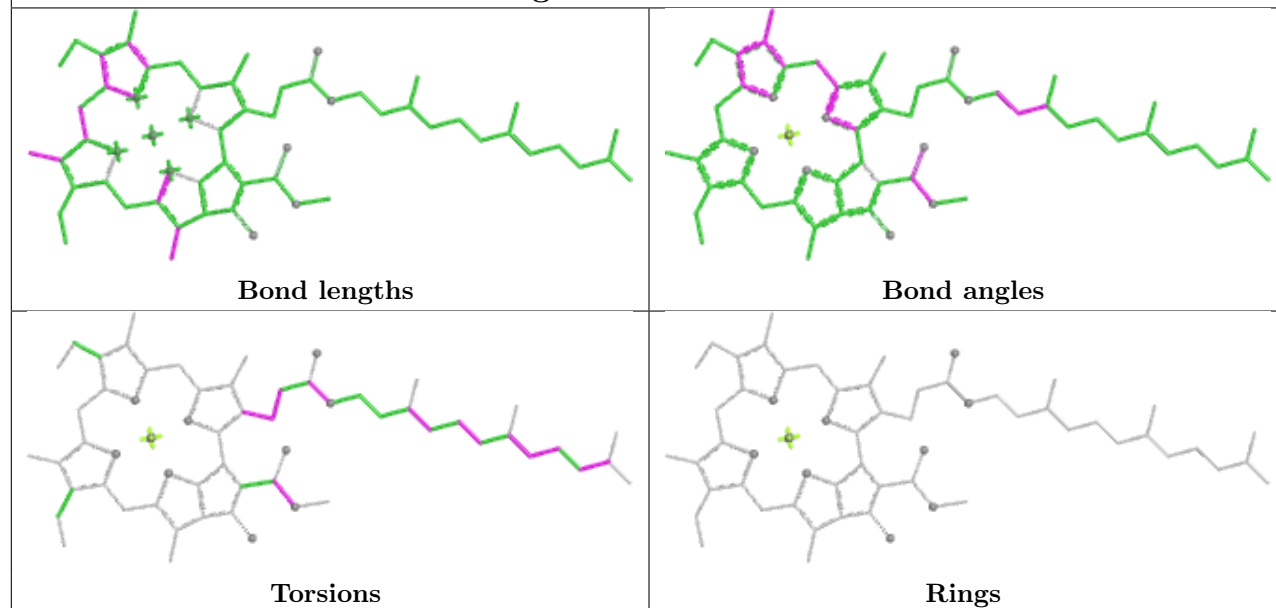
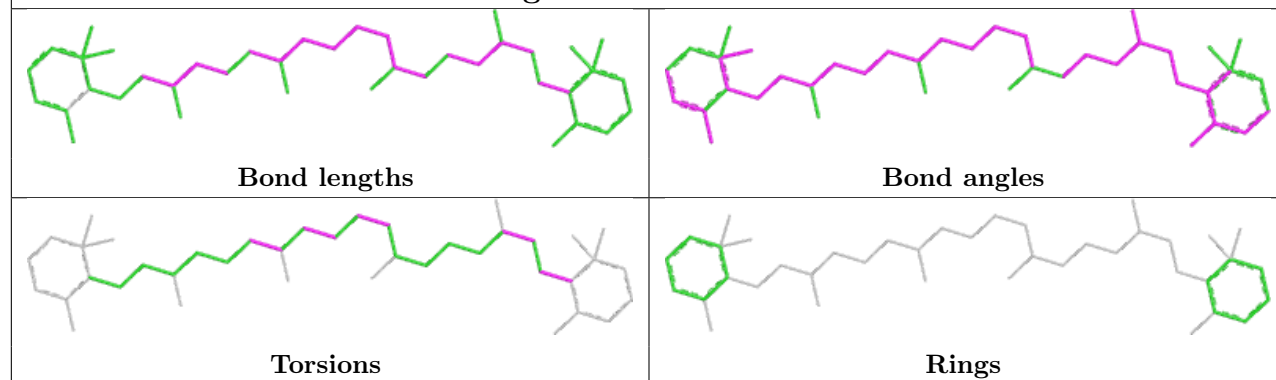
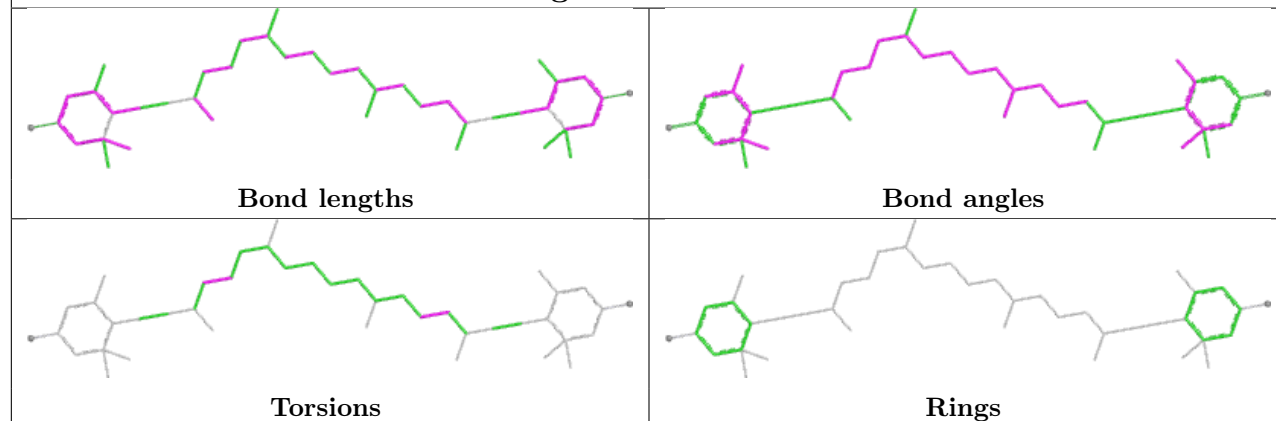
## Ligand CLA B 827

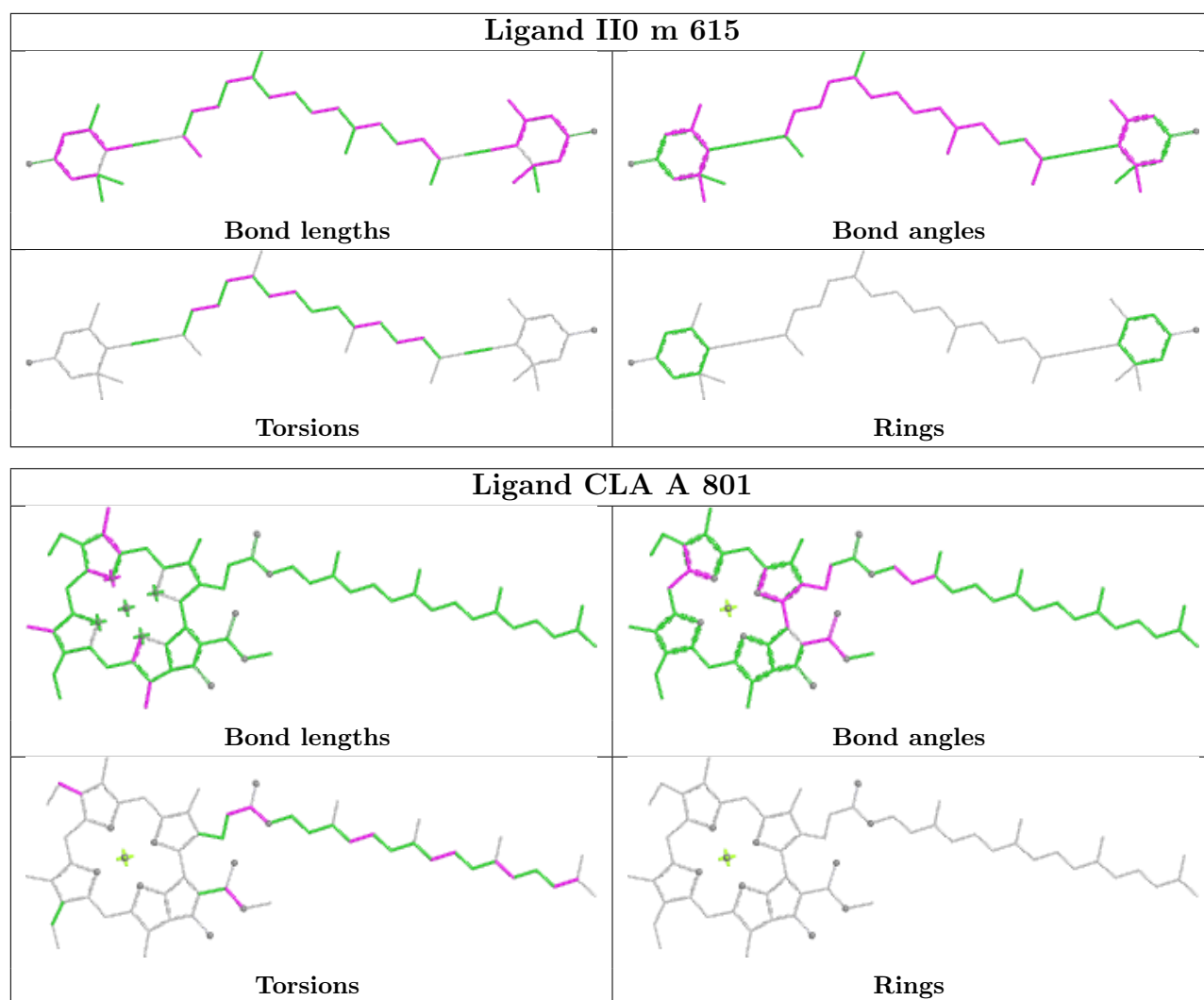


## Ligand CLA A 839

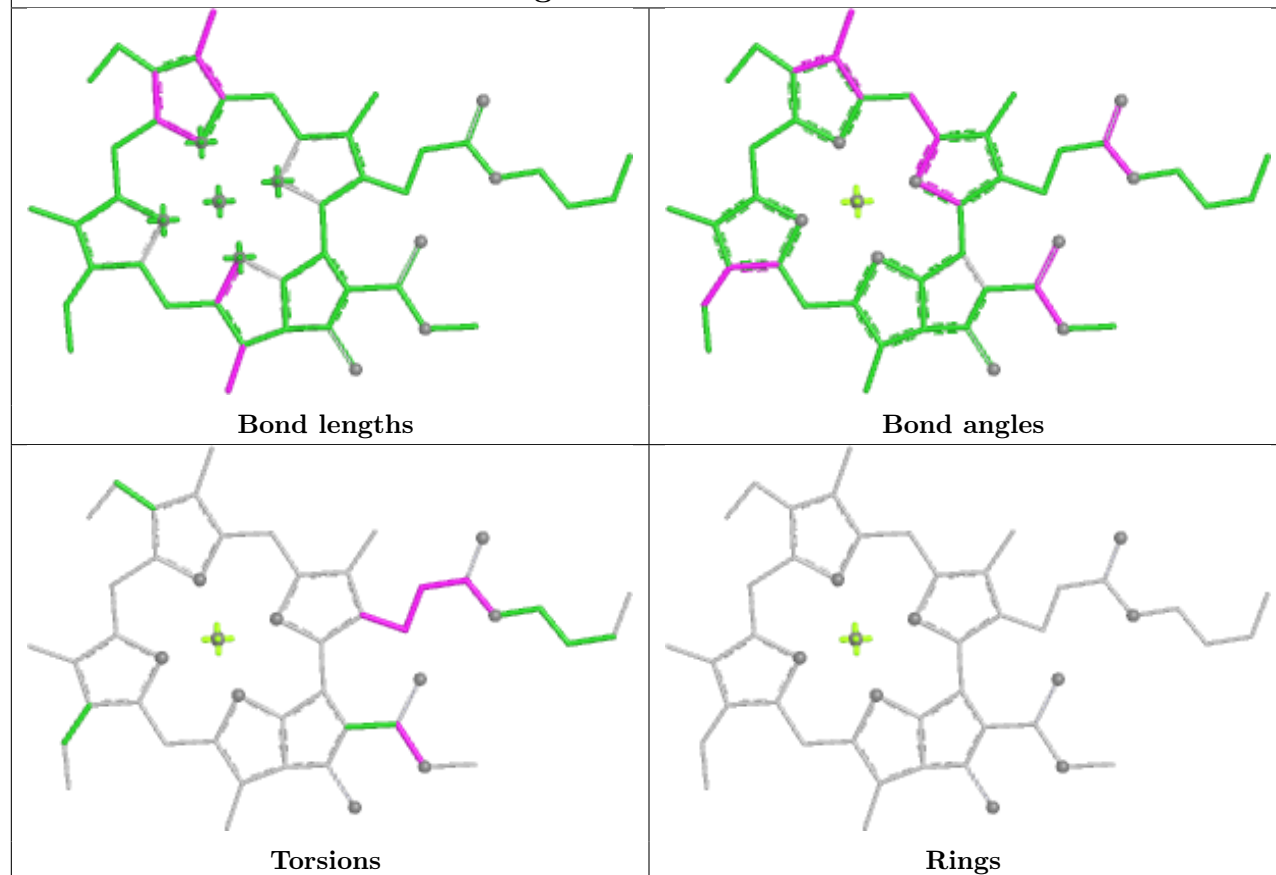


**Ligand CLA h 313****Ligand CLA A 831**

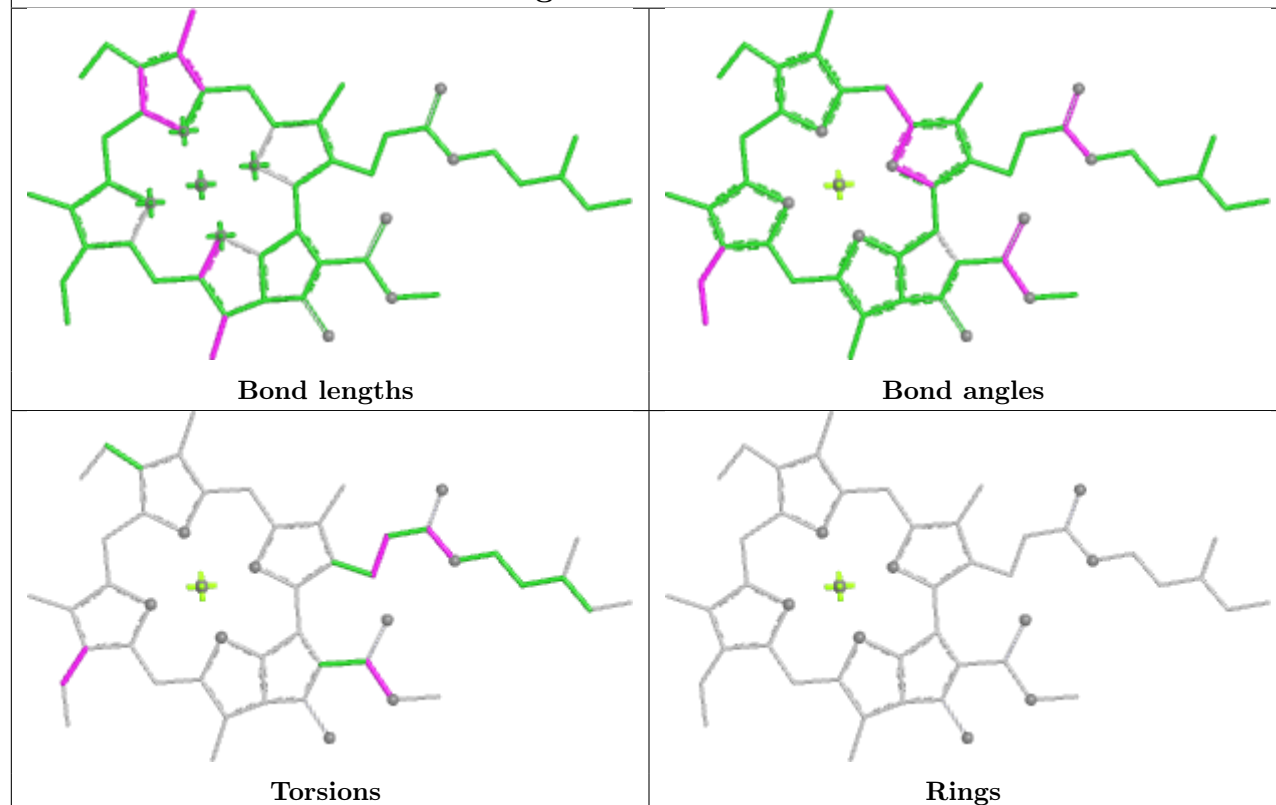
**Ligand CLA B 813****Ligand WVN A 849****Ligand II0 a 315**

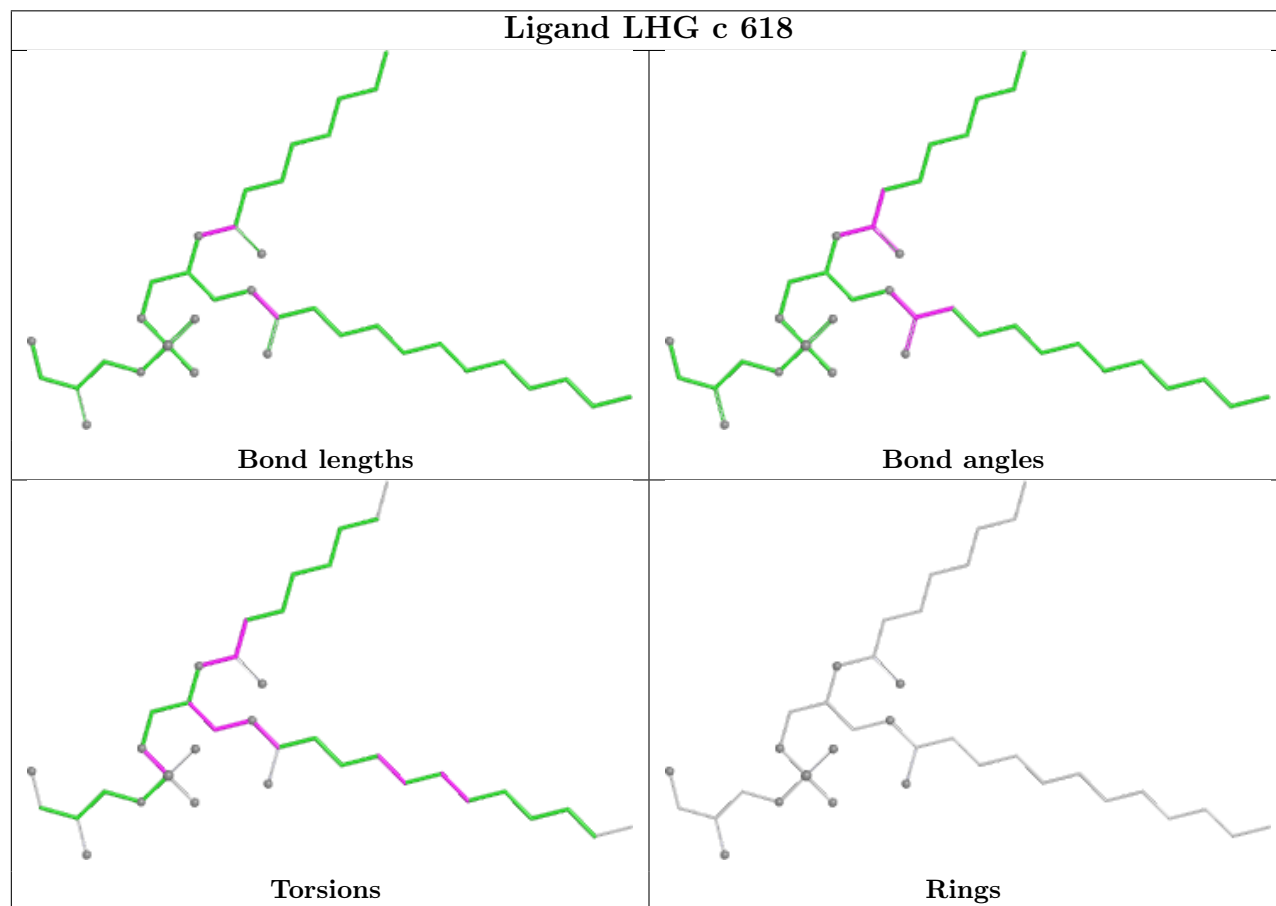
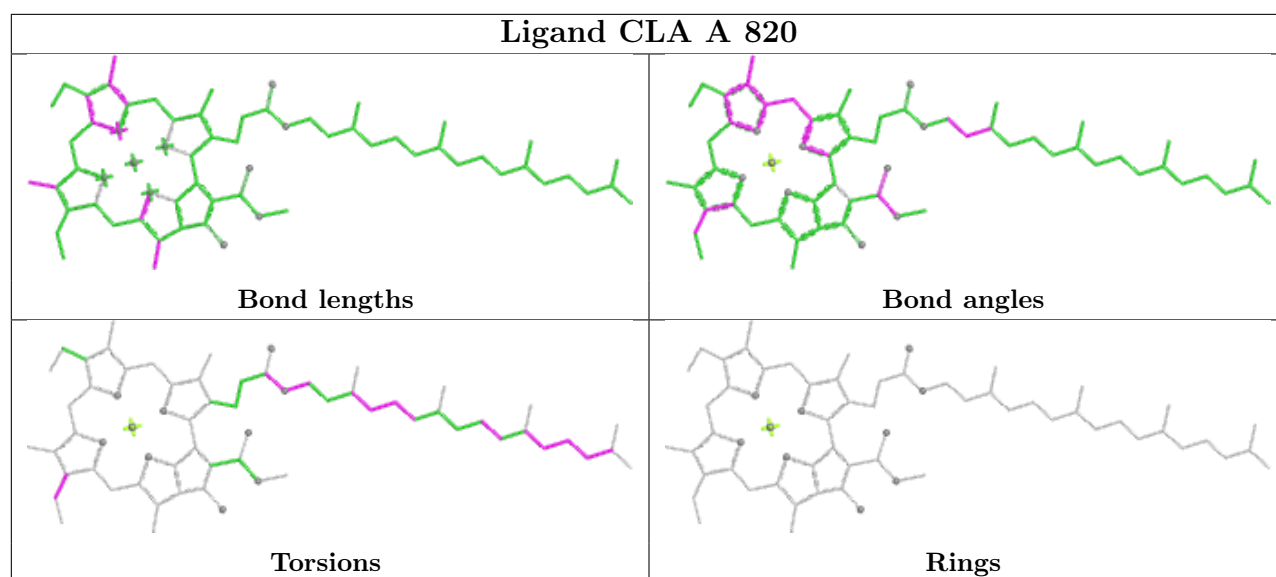


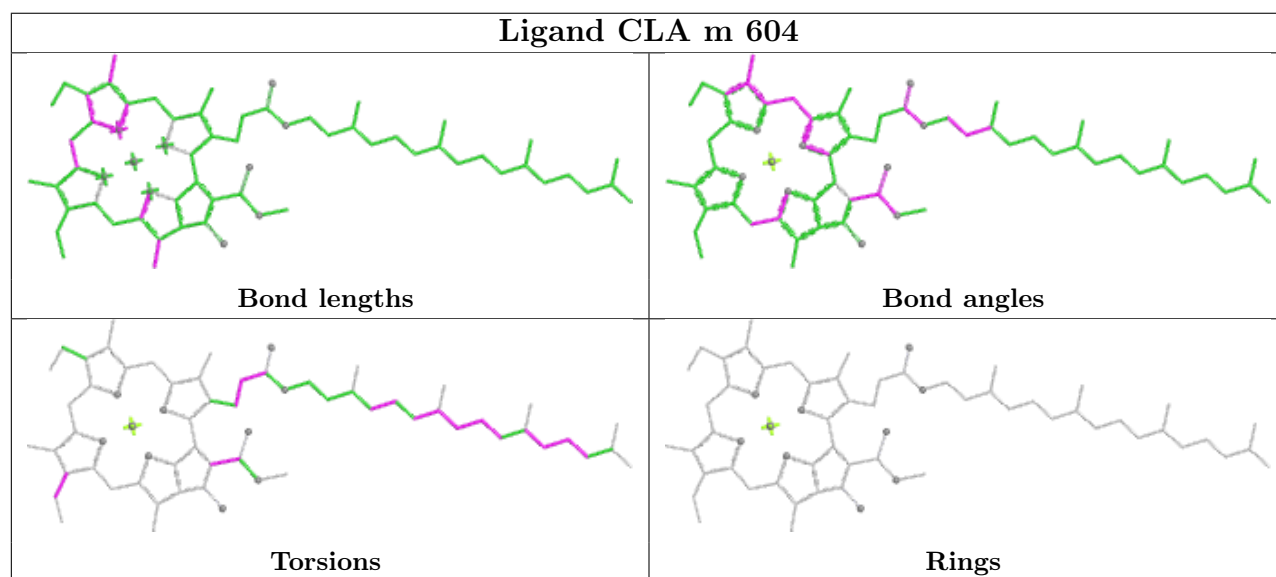
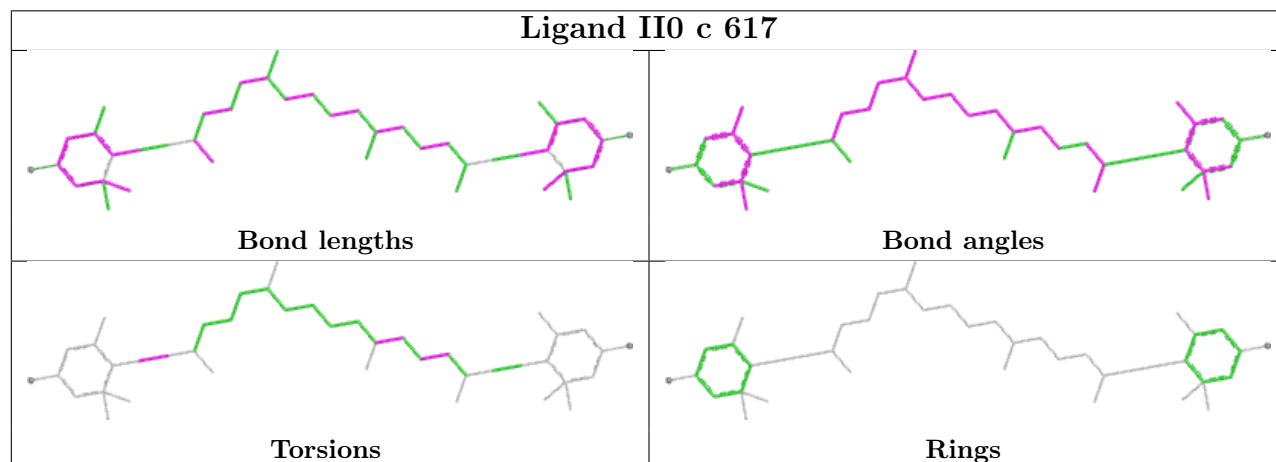
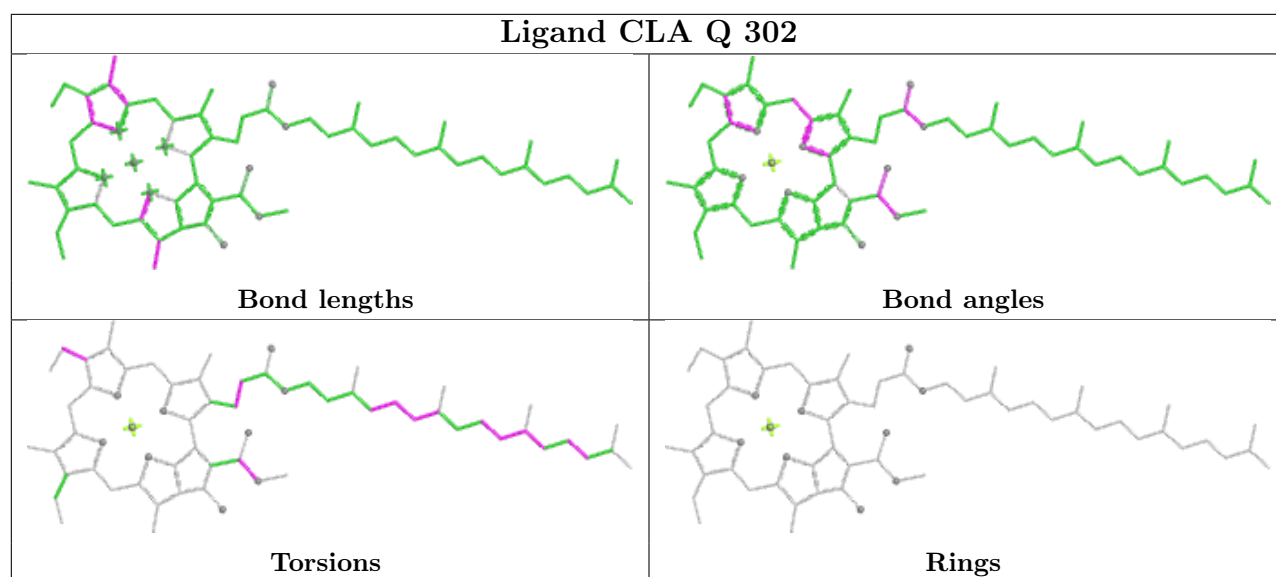
## Ligand CLA L 202

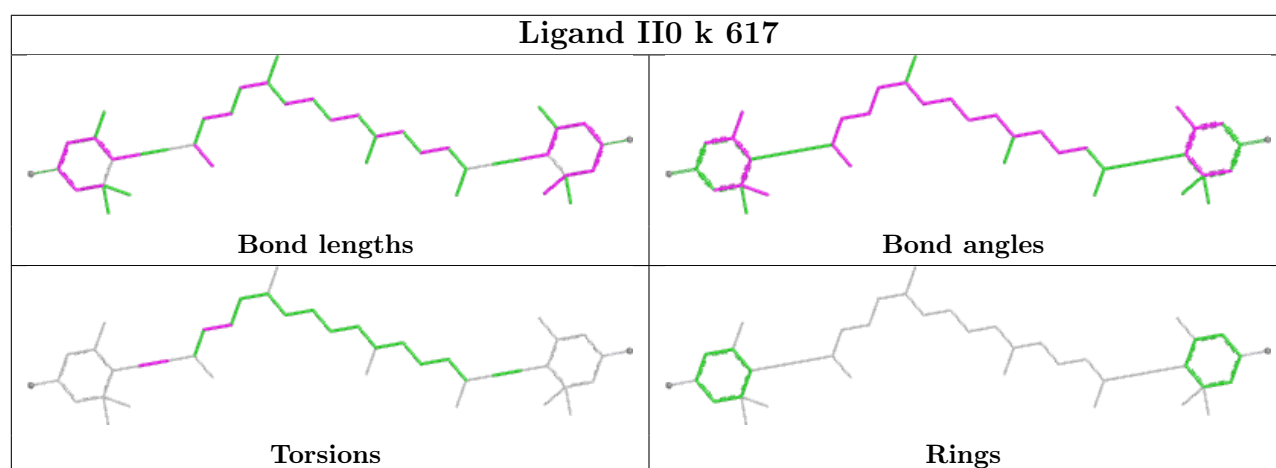
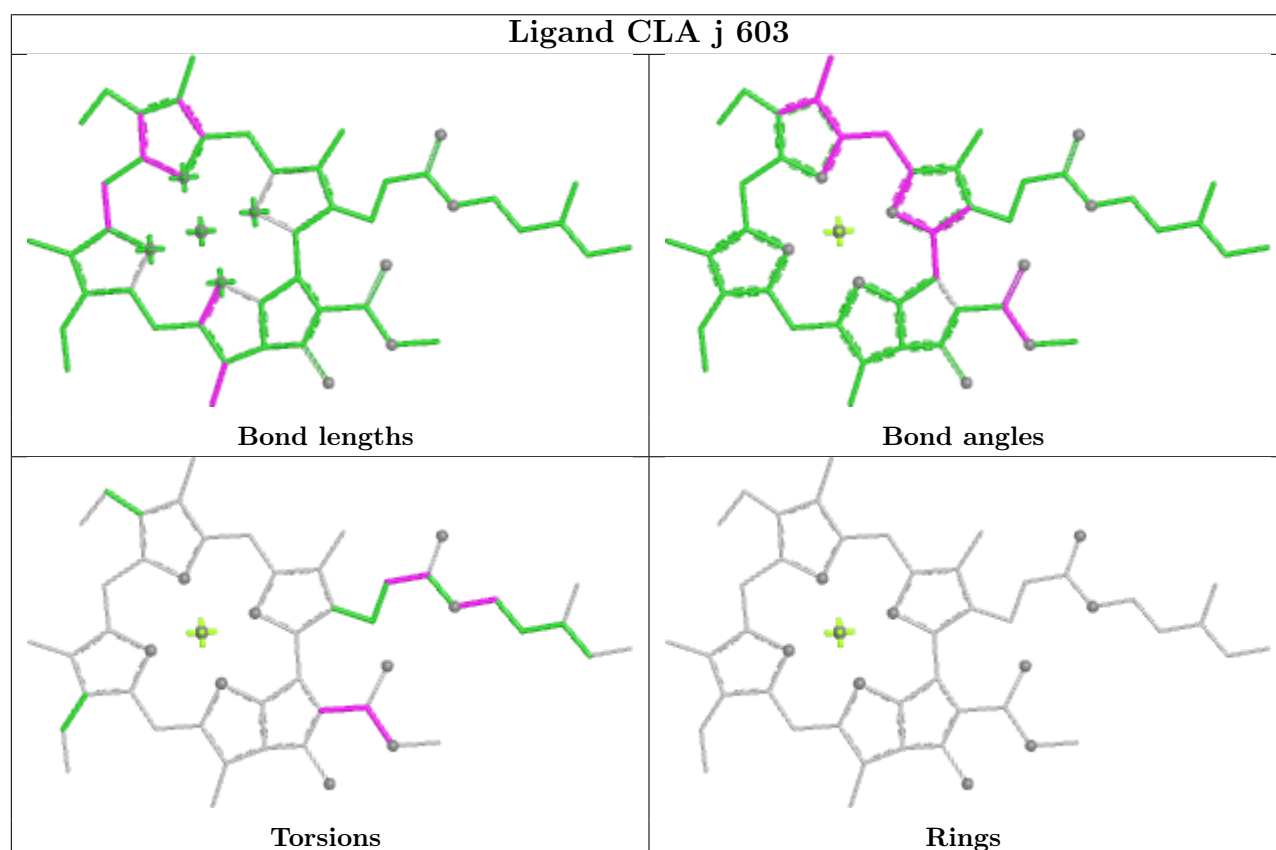
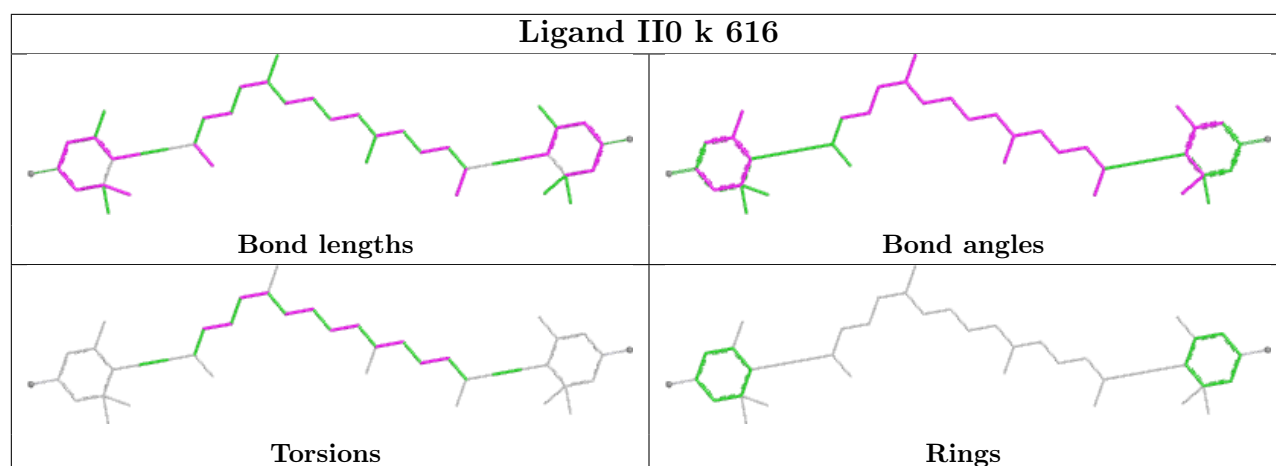


## Ligand CLA k 601

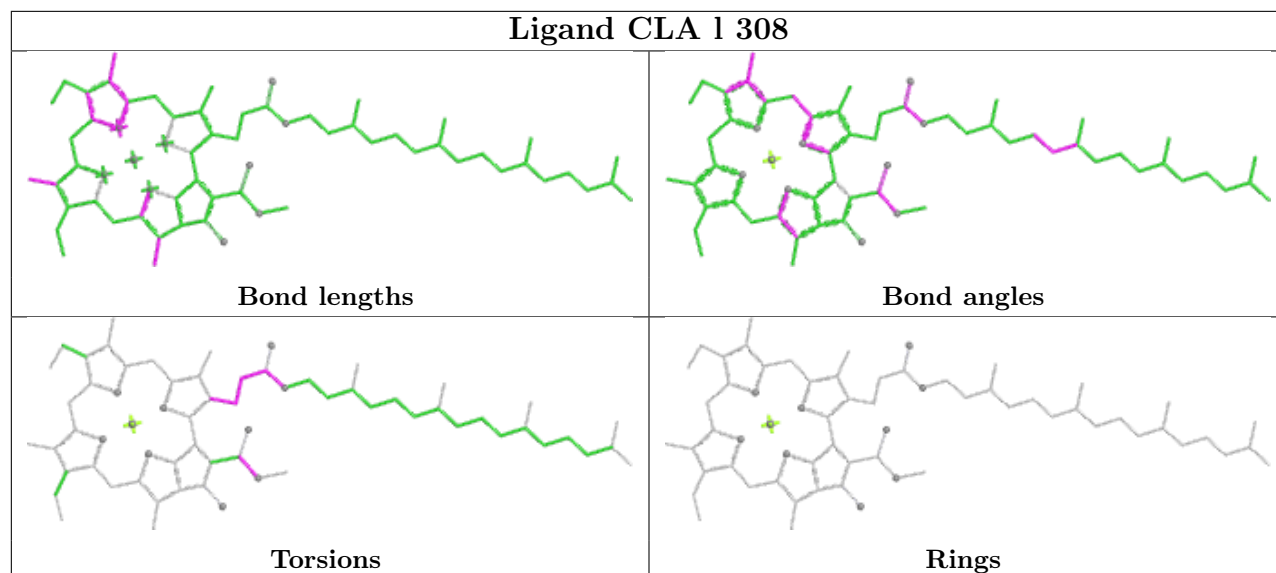
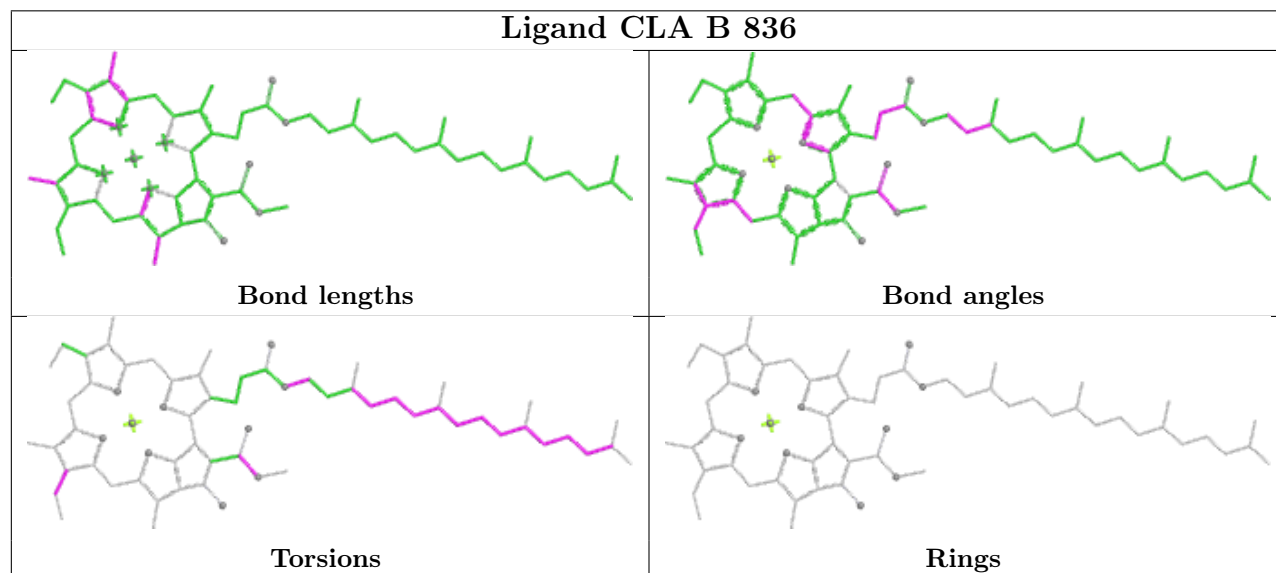
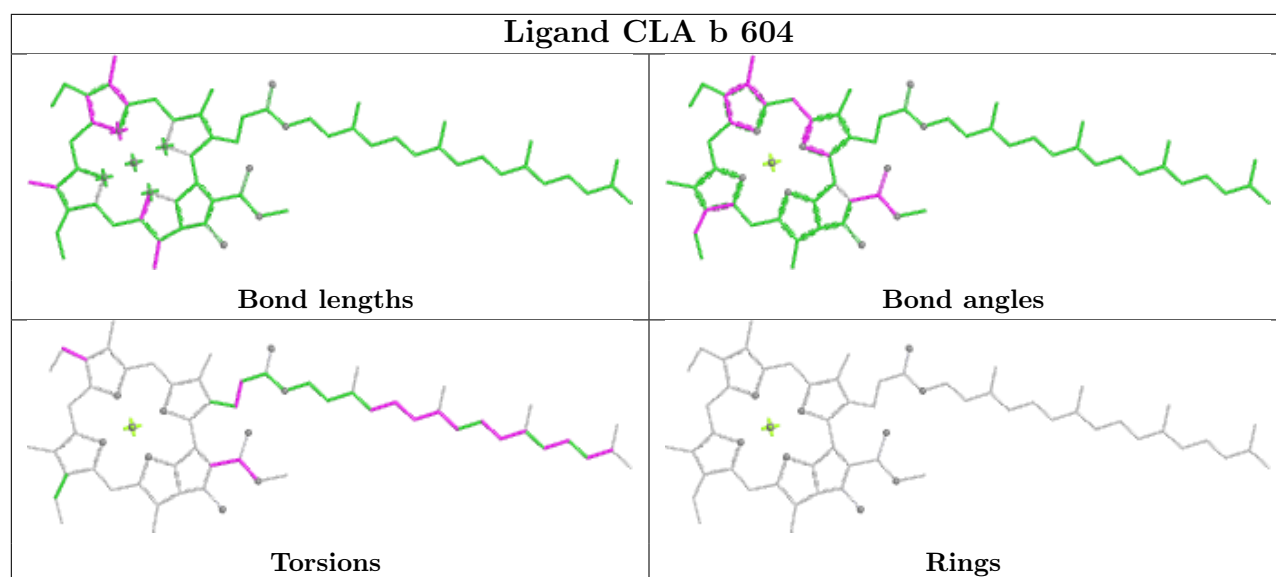




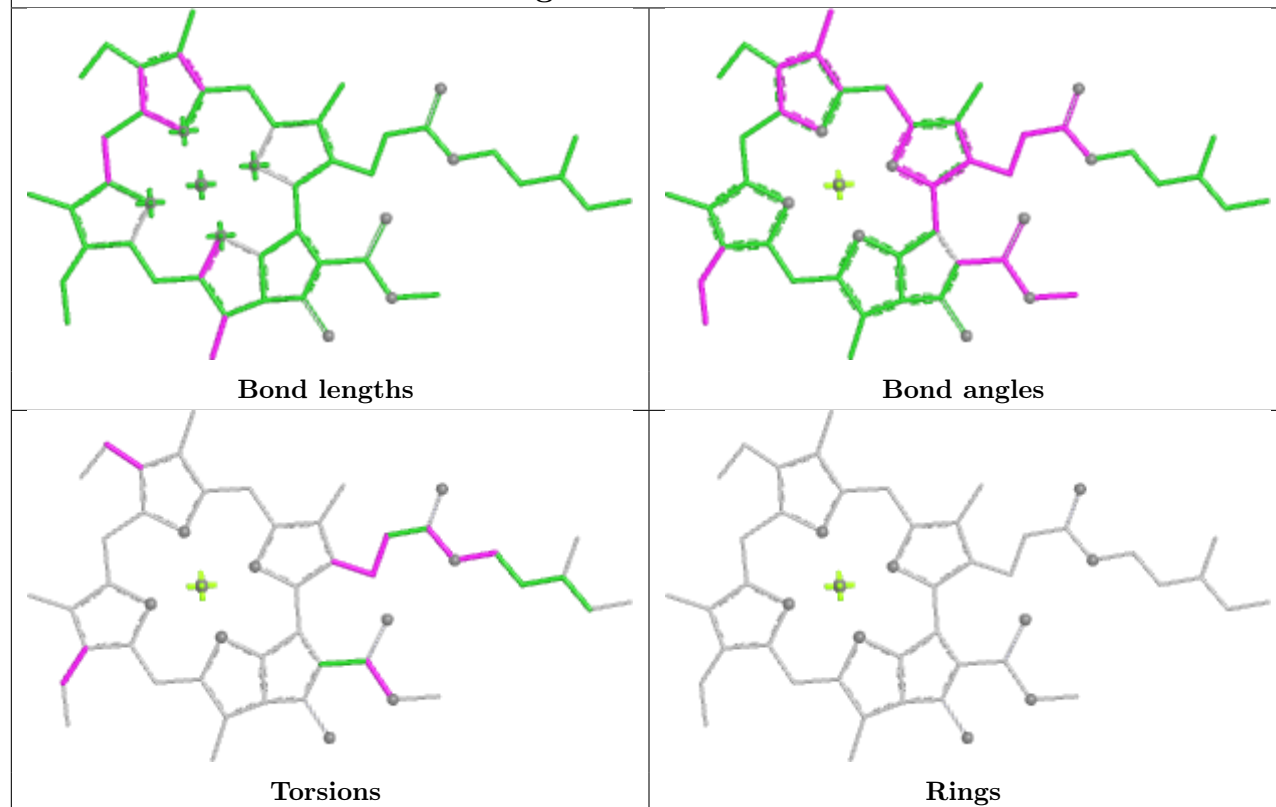




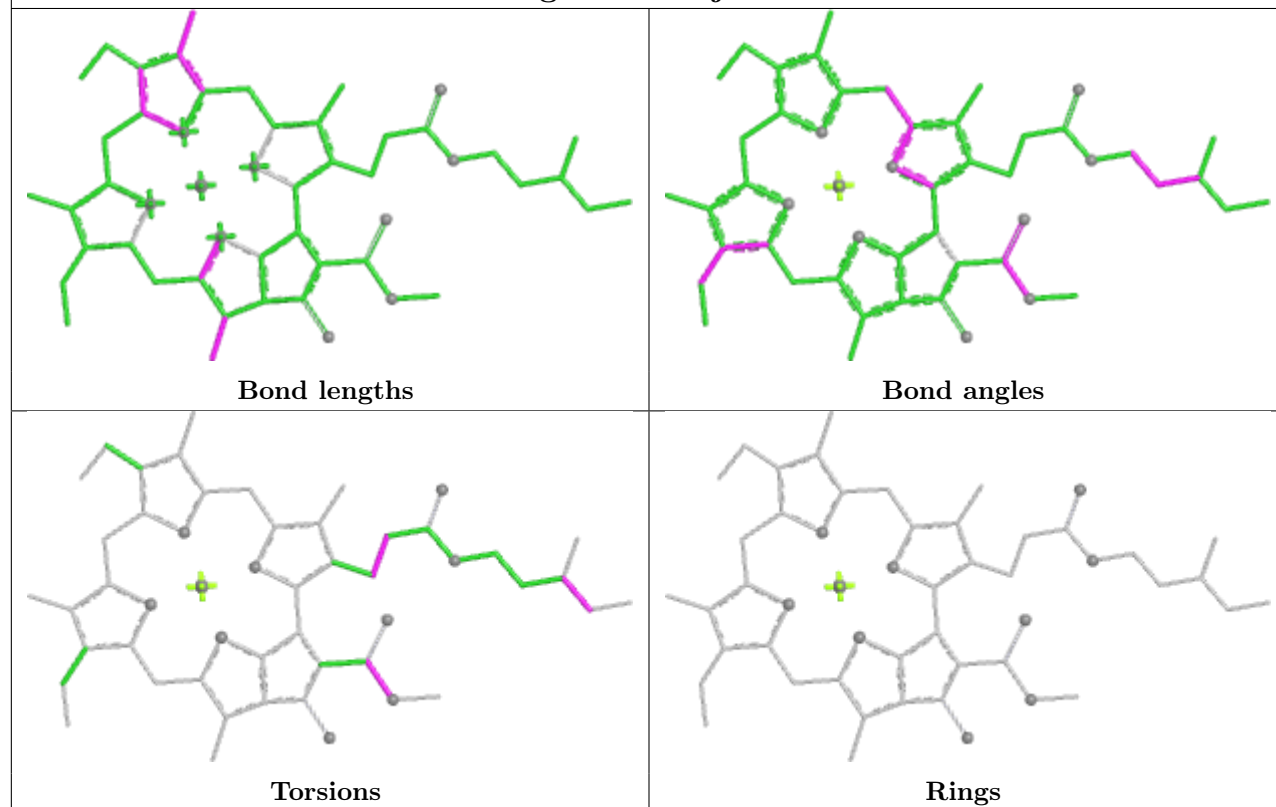


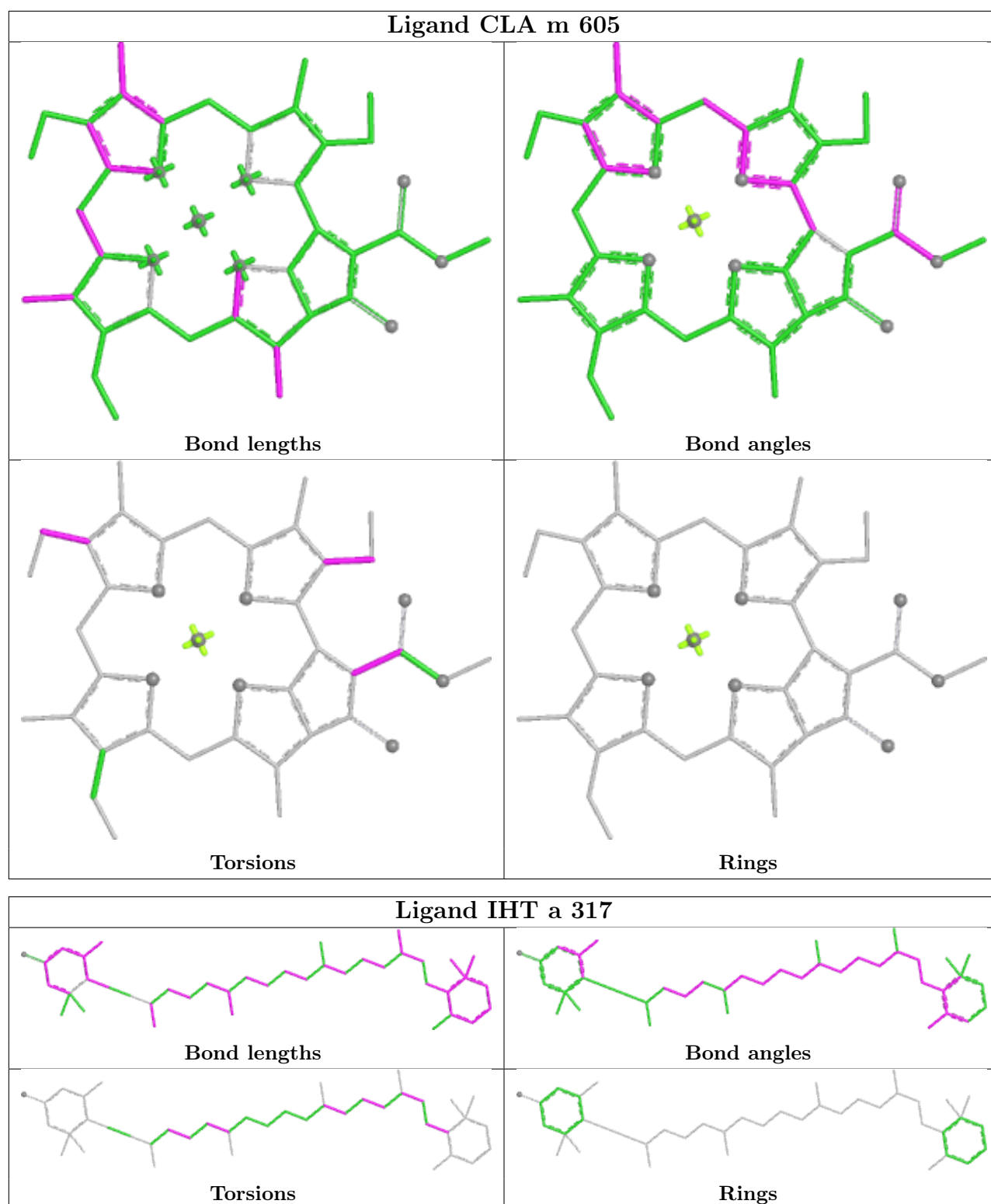


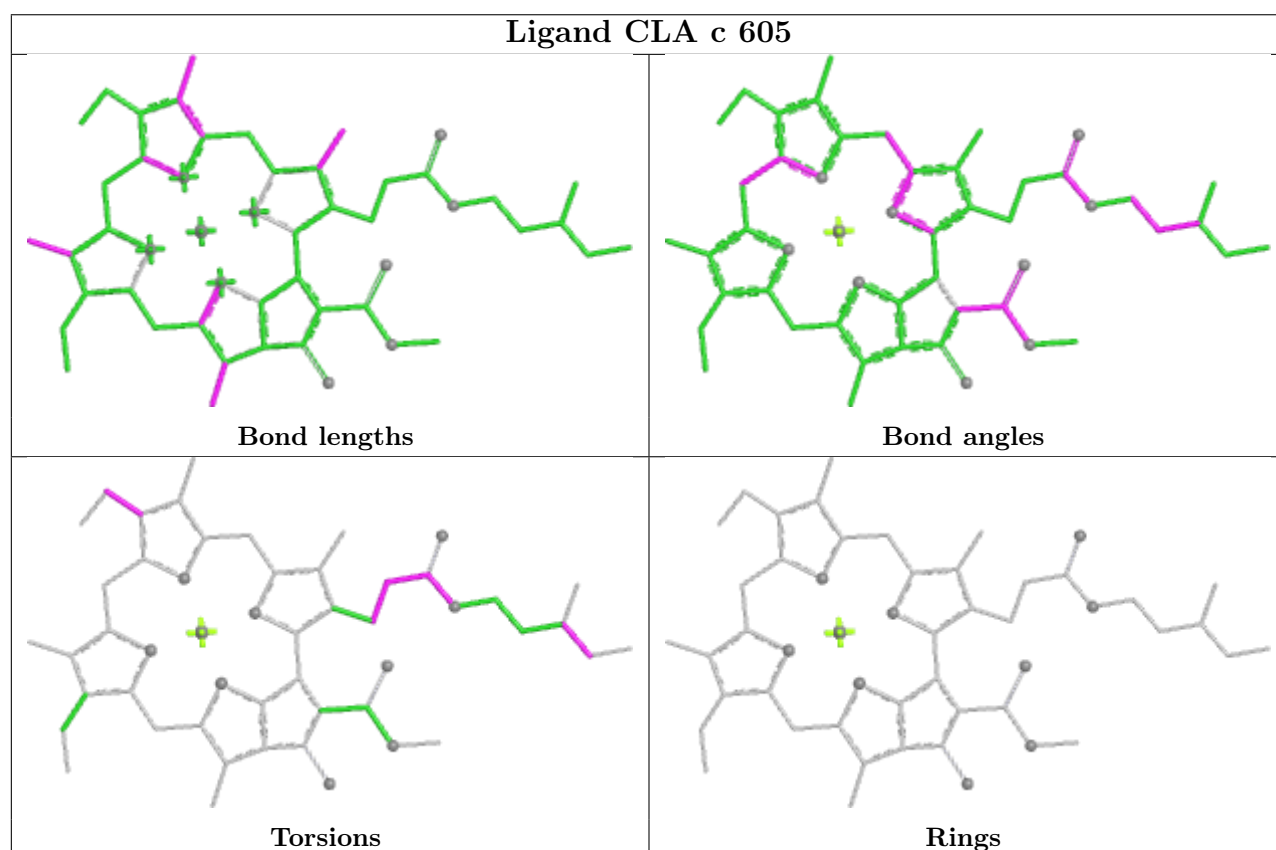
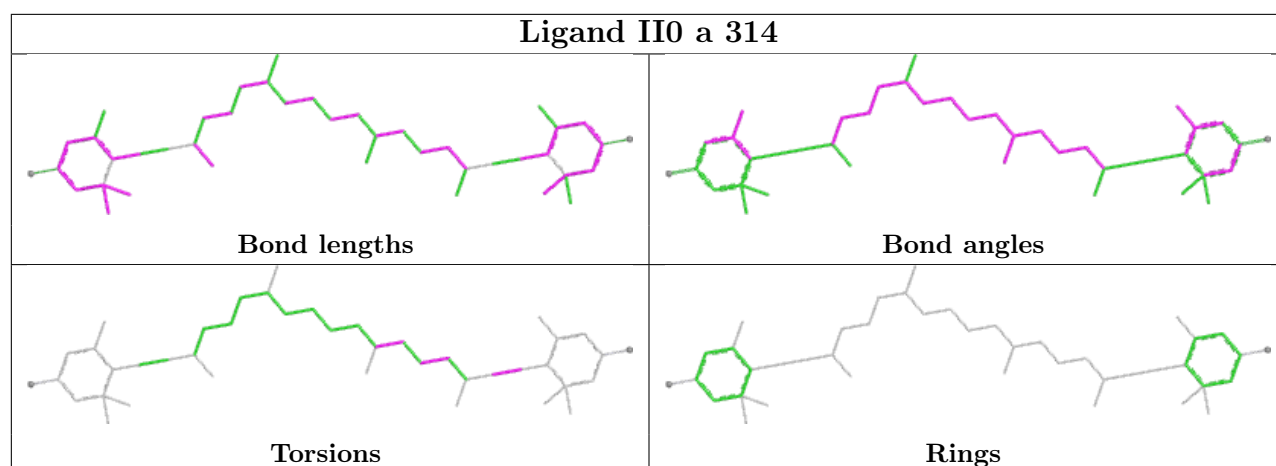
## Ligand CLA k 614



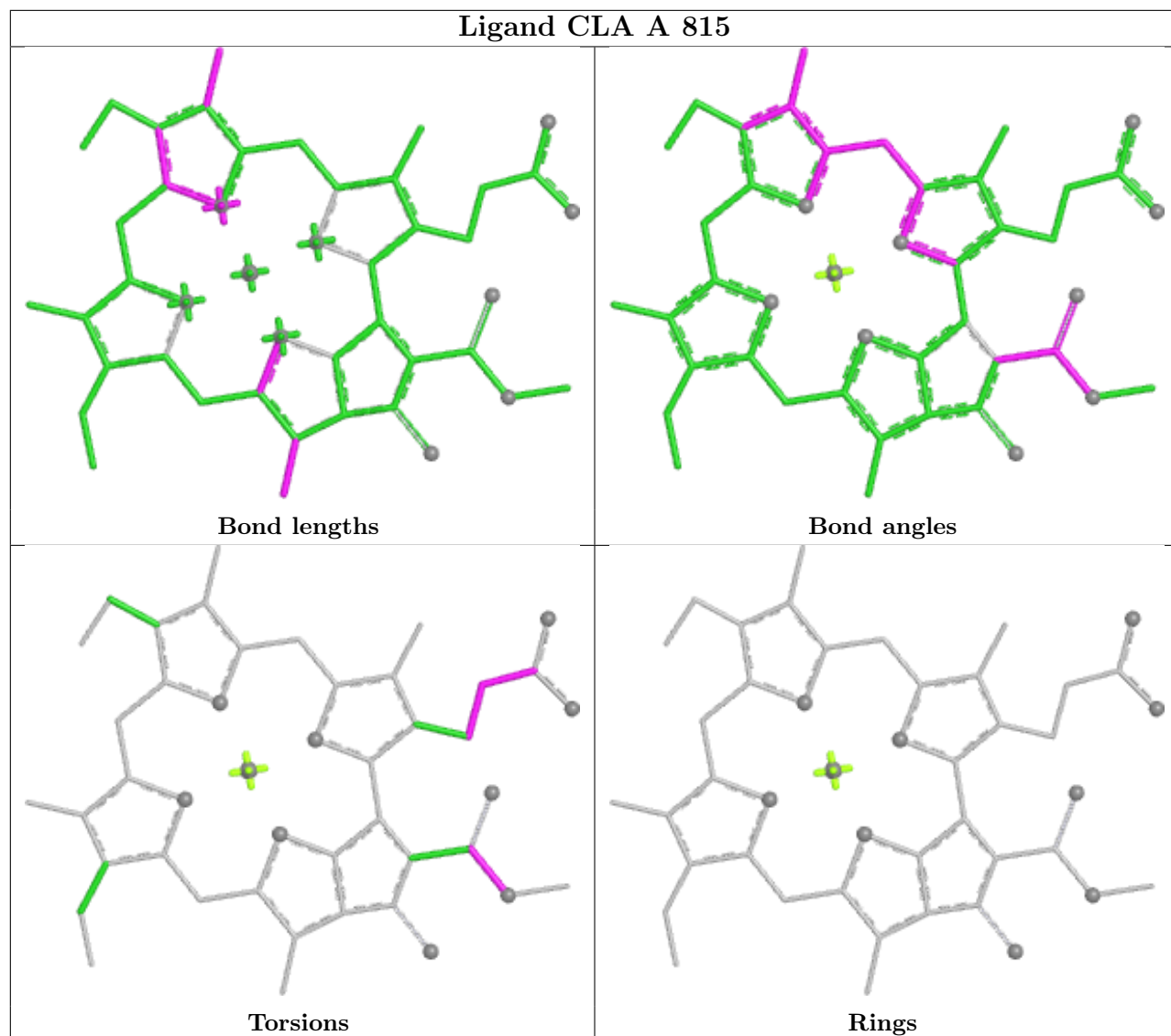
## Ligand CLA j 601



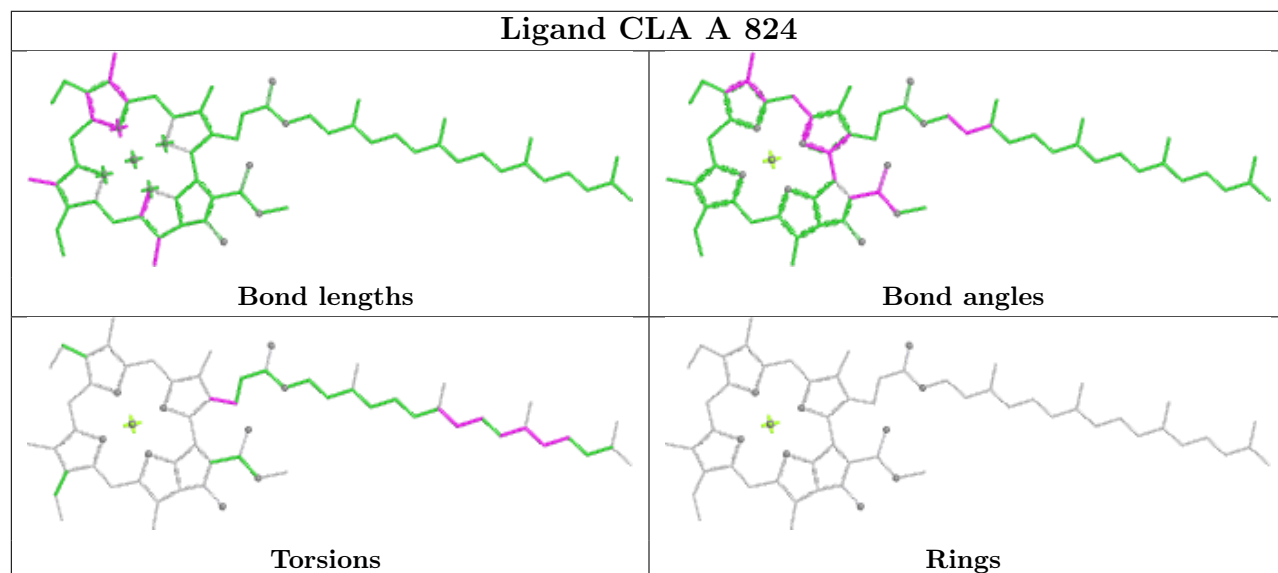




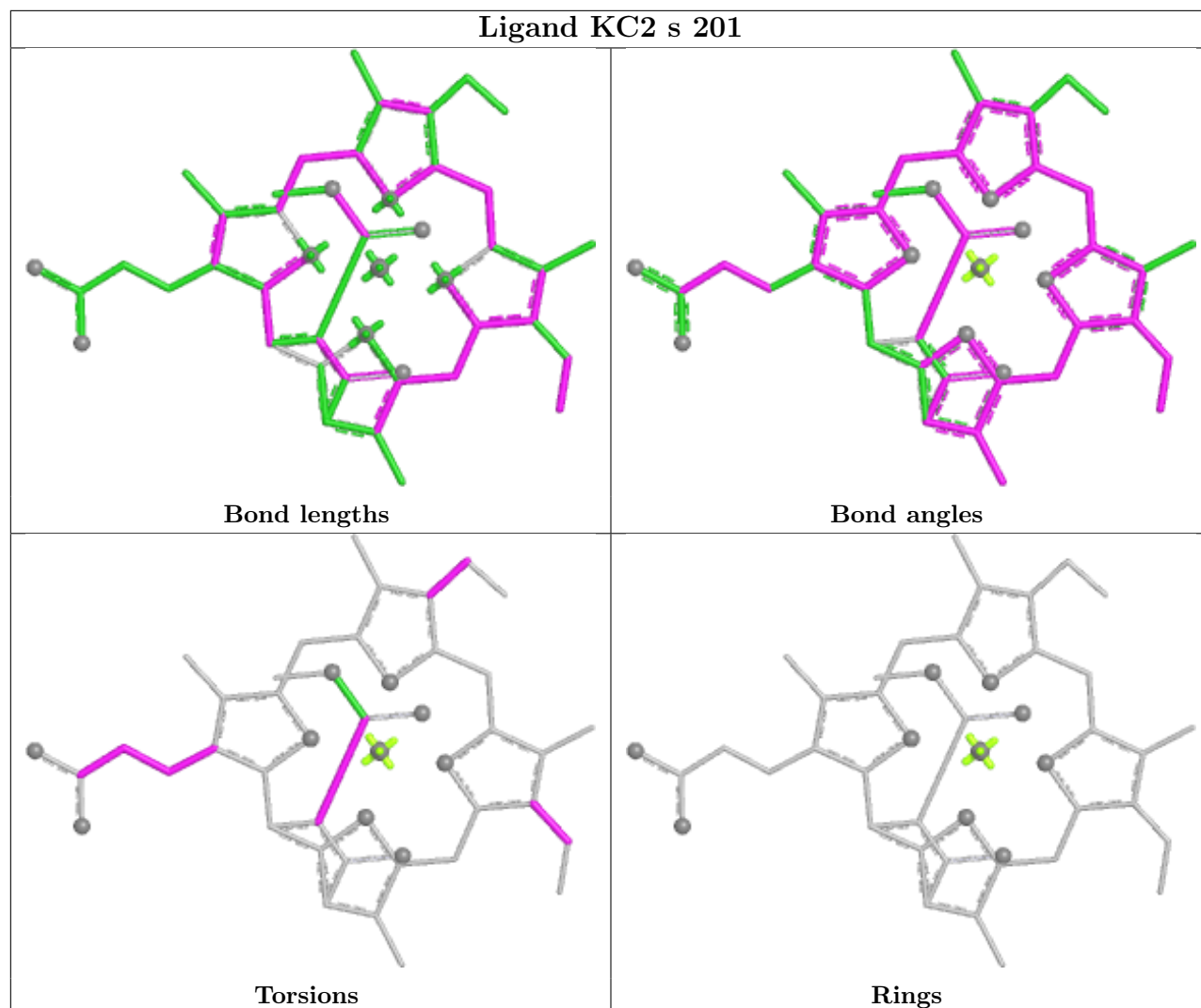
## Ligand CLA A 815



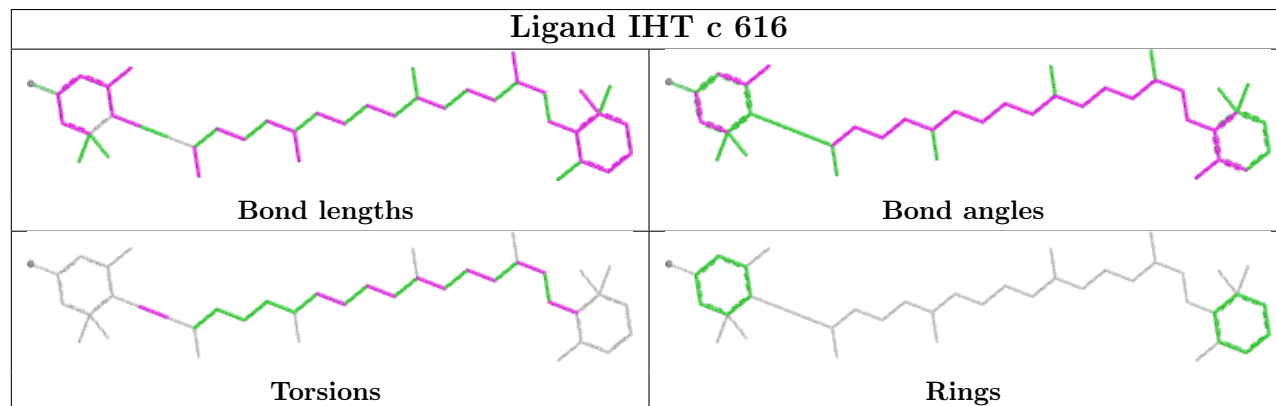
## Ligand CLA A 824

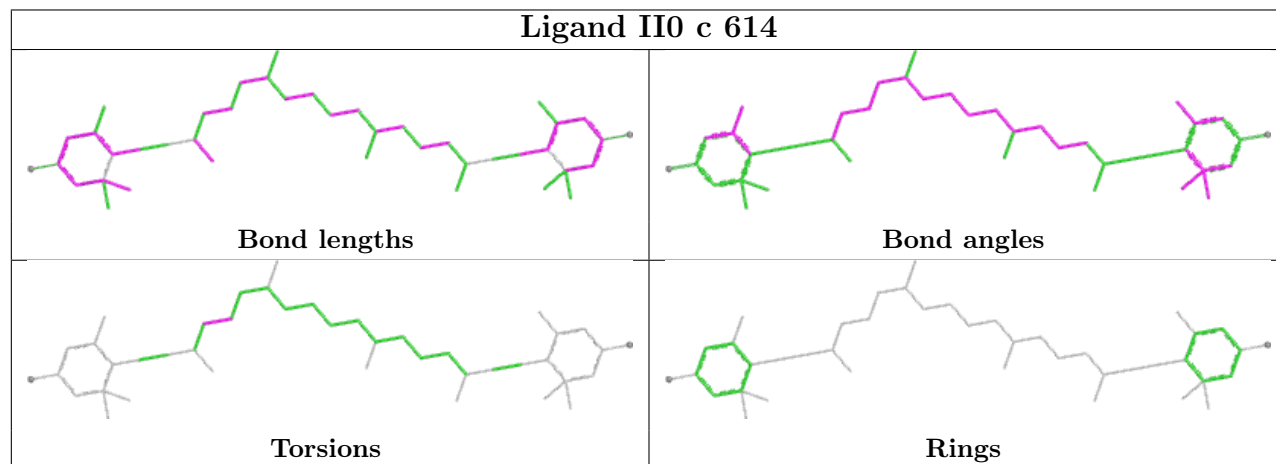
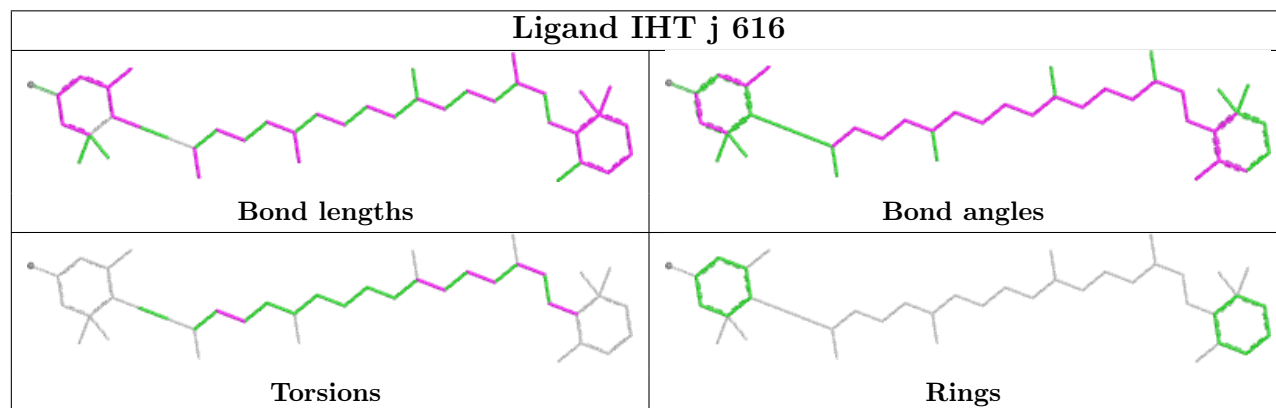
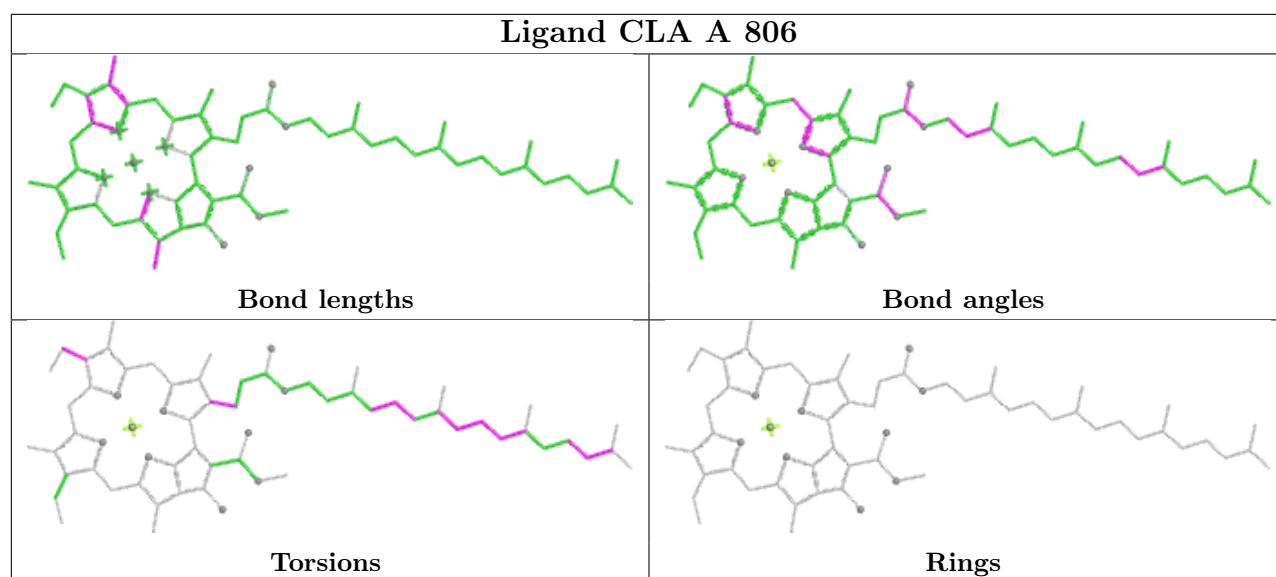


## Ligand KC2 s 201

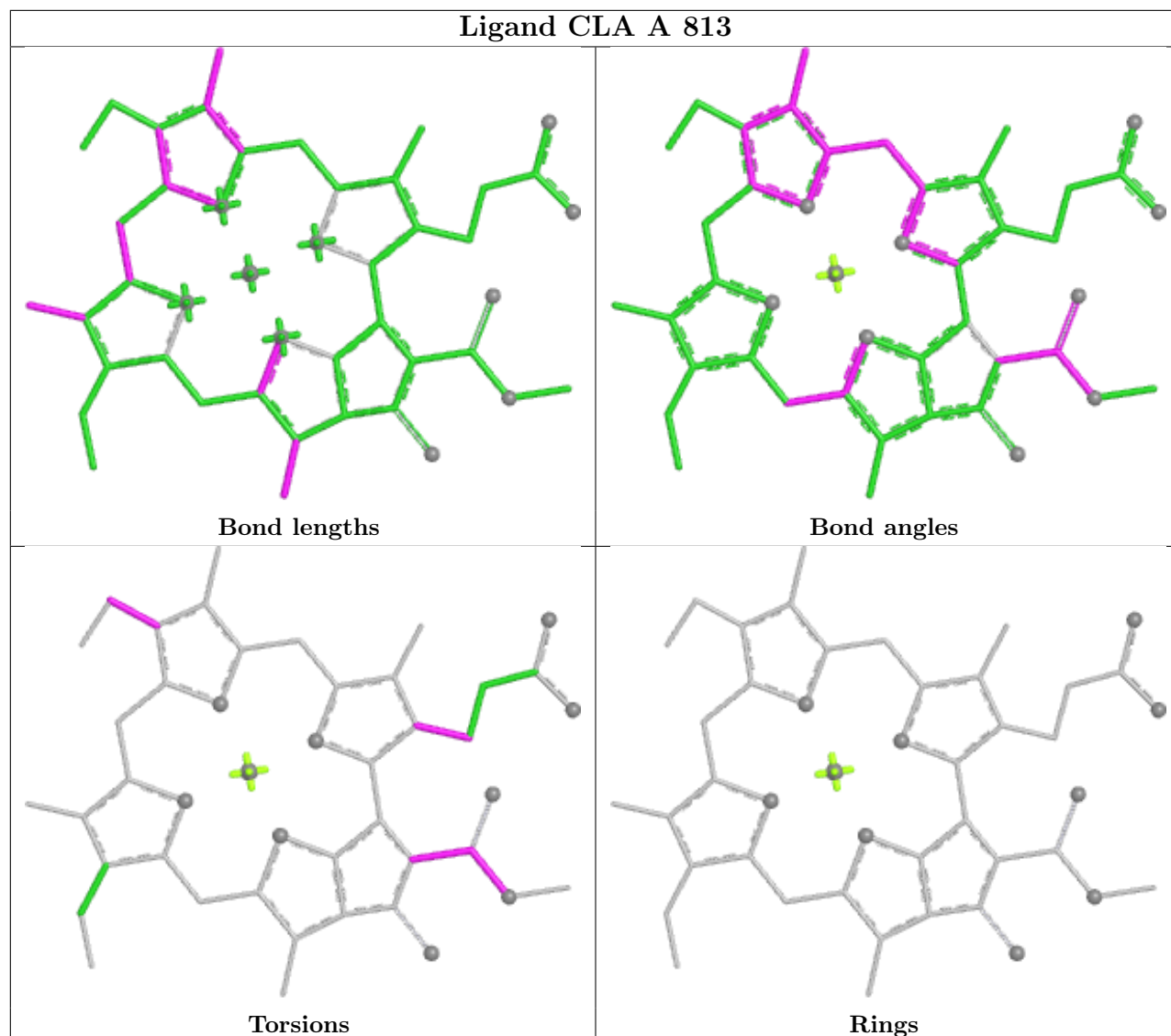


## Ligand IHT c 616

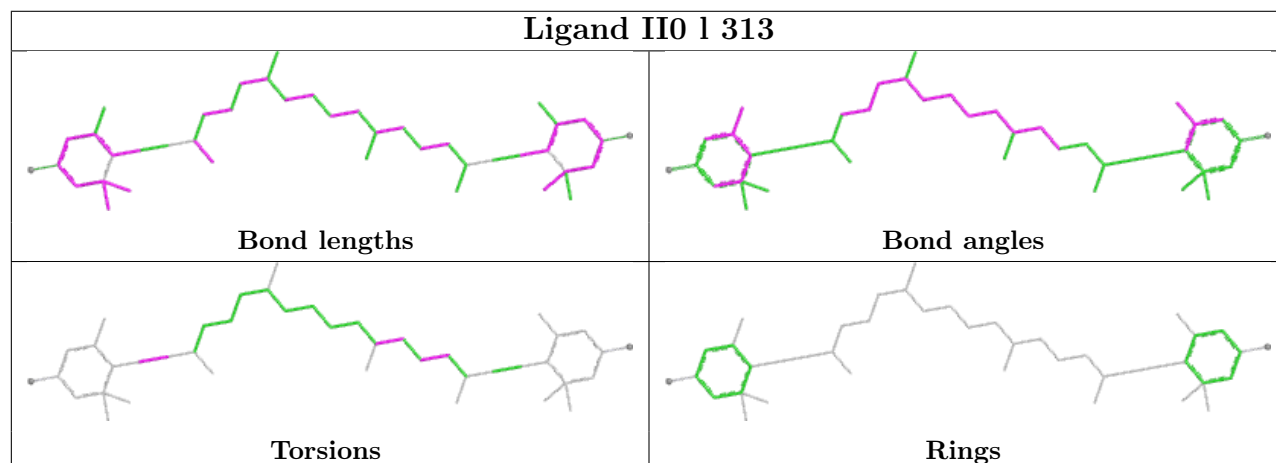




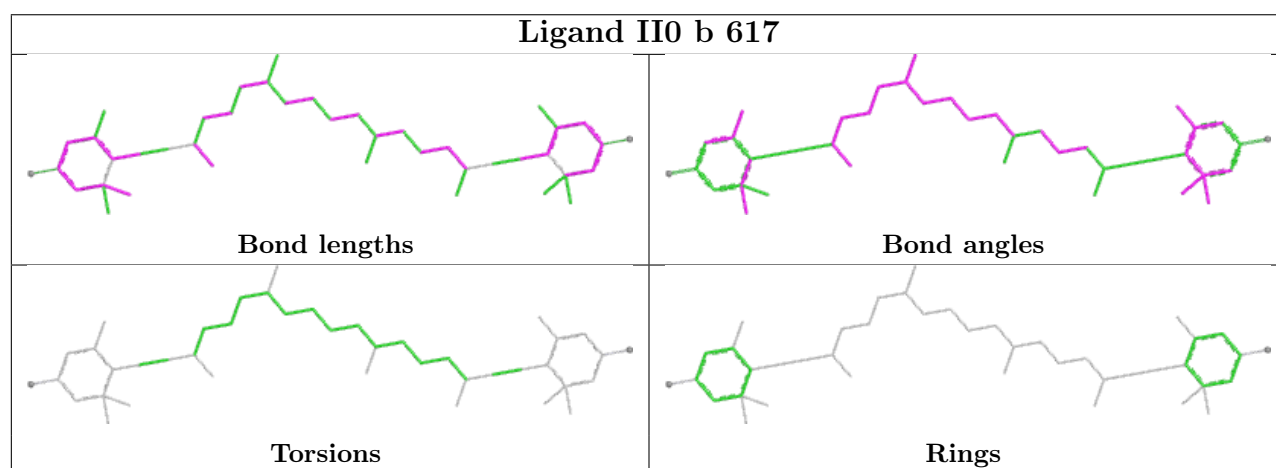
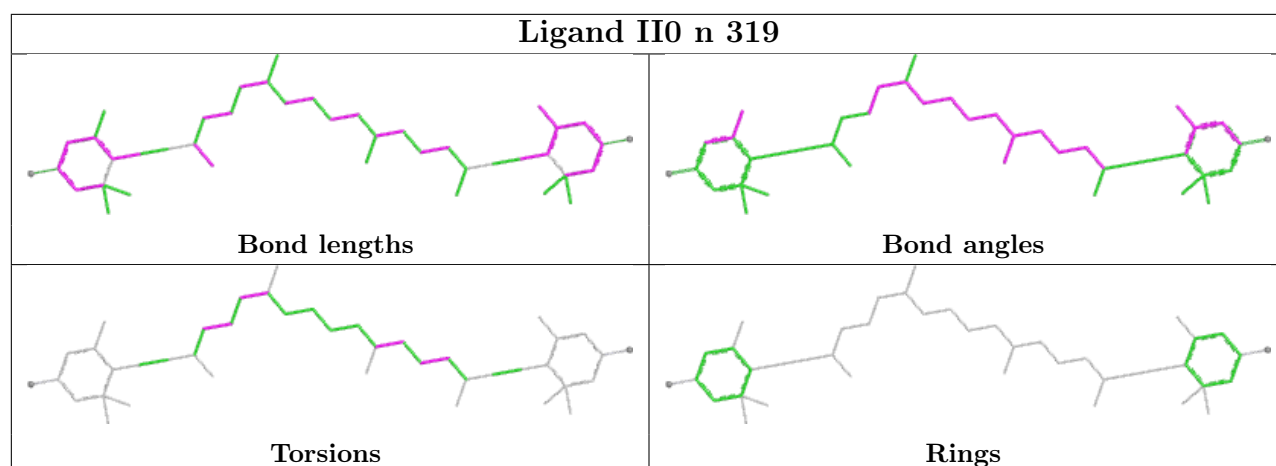
## Ligand CLA A 813



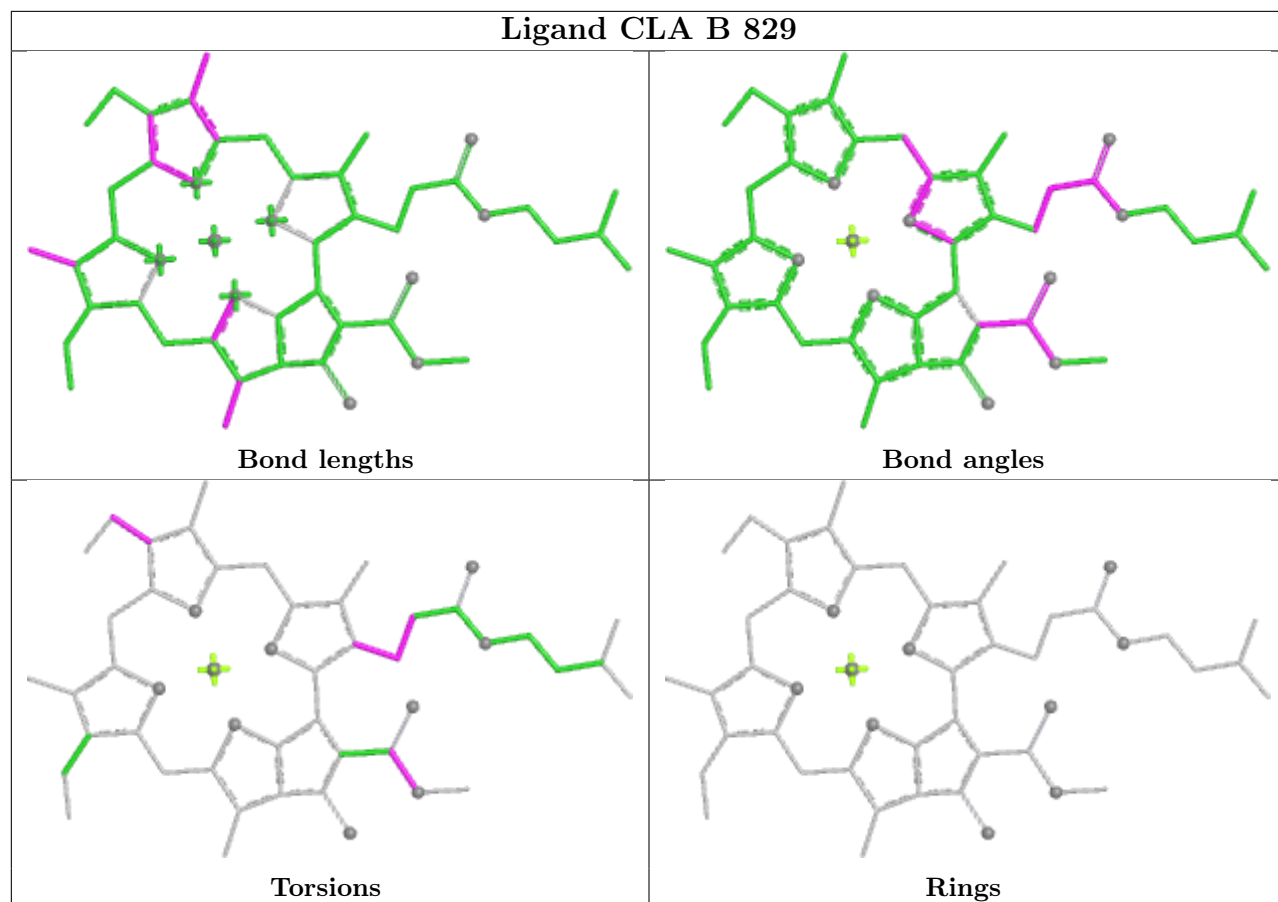
## Ligand II0 1 313



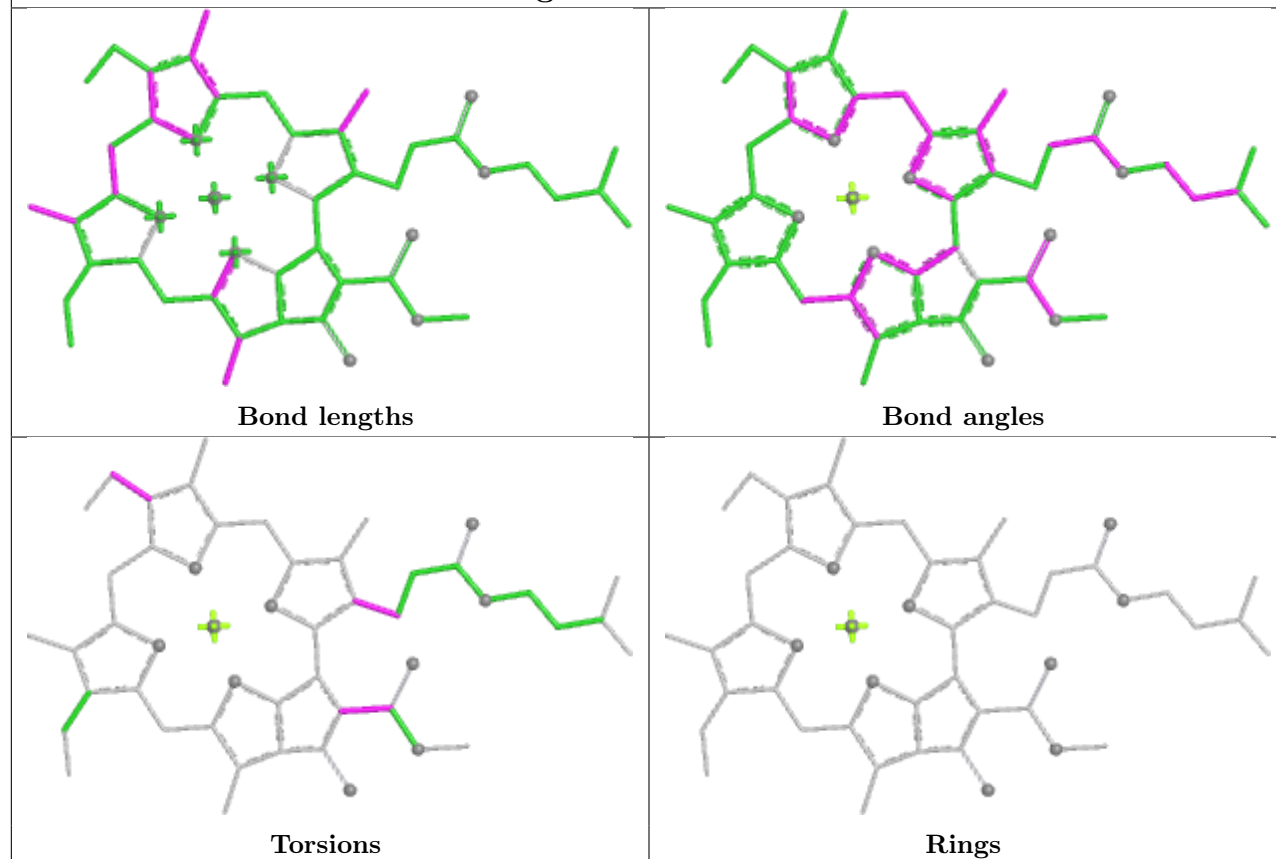




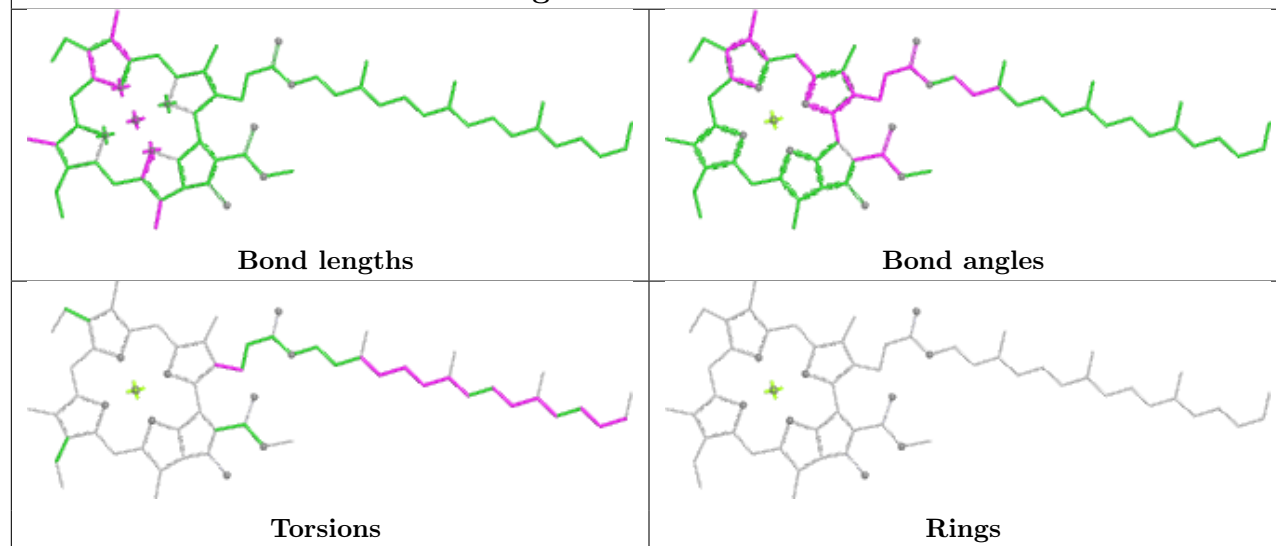
## Ligand CLA B 829

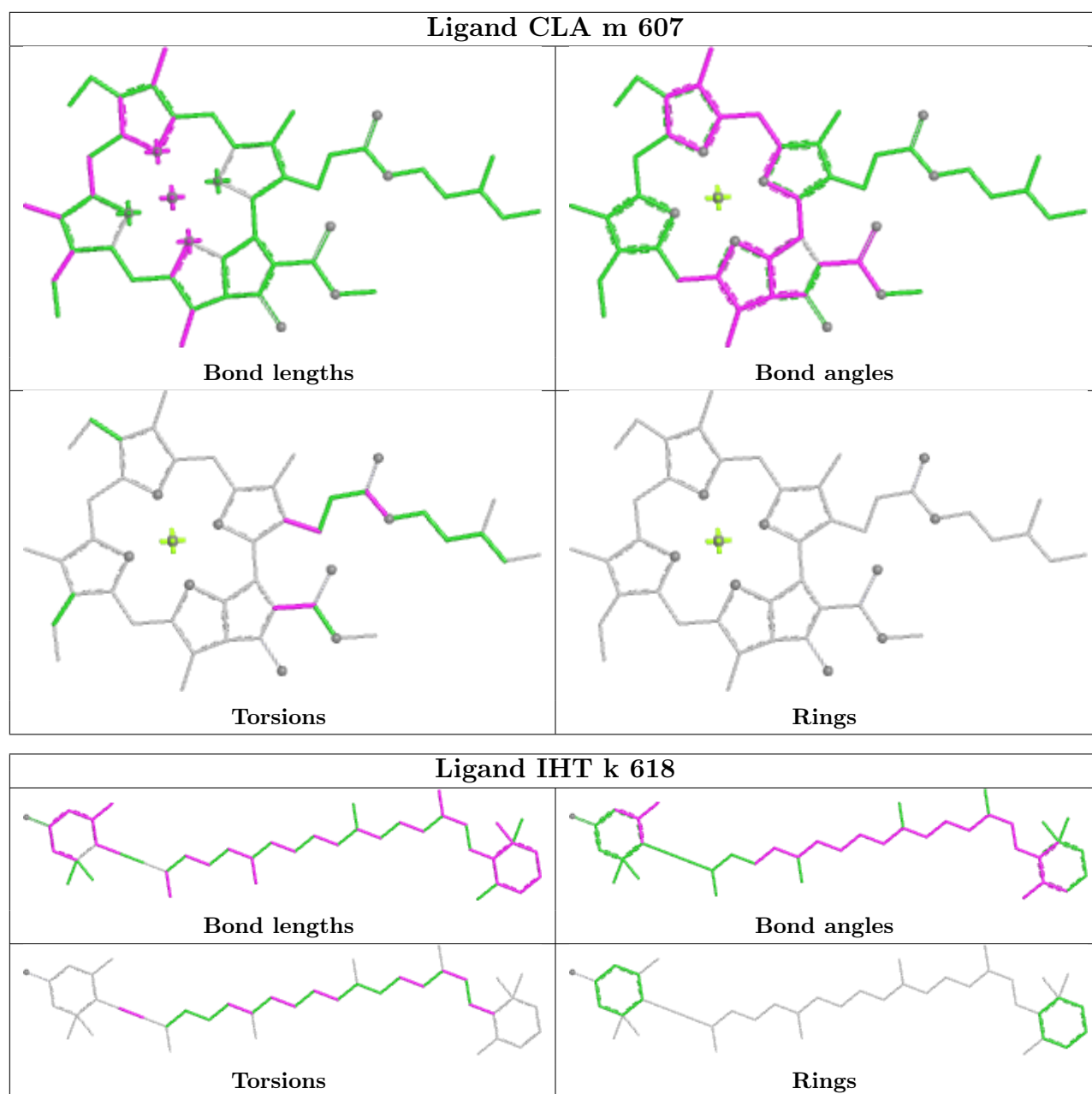


## Ligand CLA a 304

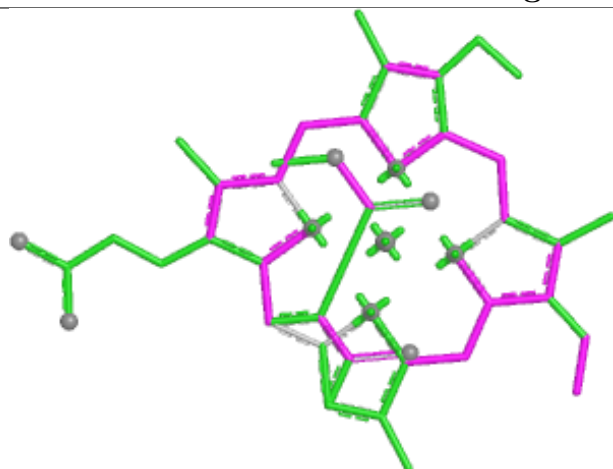


## Ligand CLA B 823

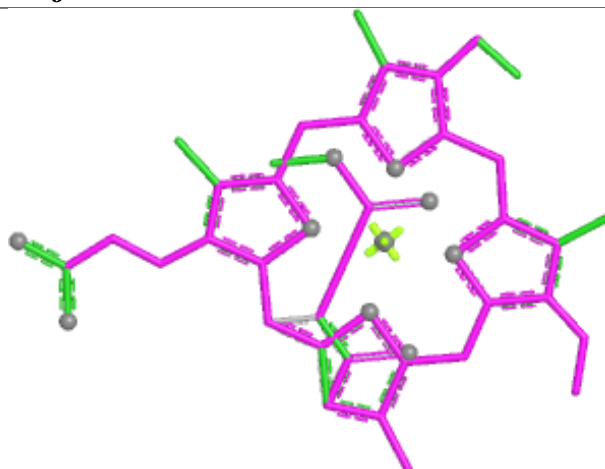




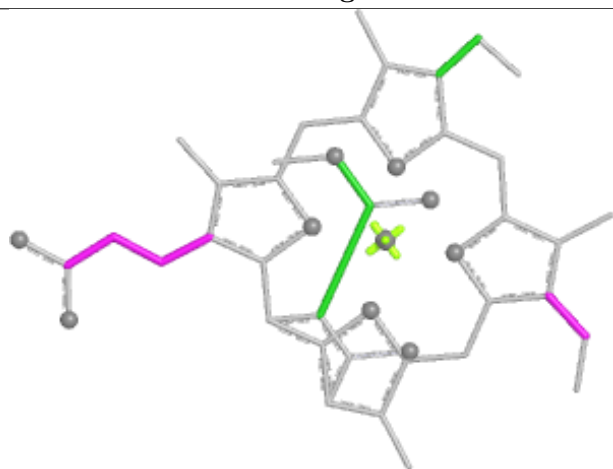
## Ligand KC2 j 610



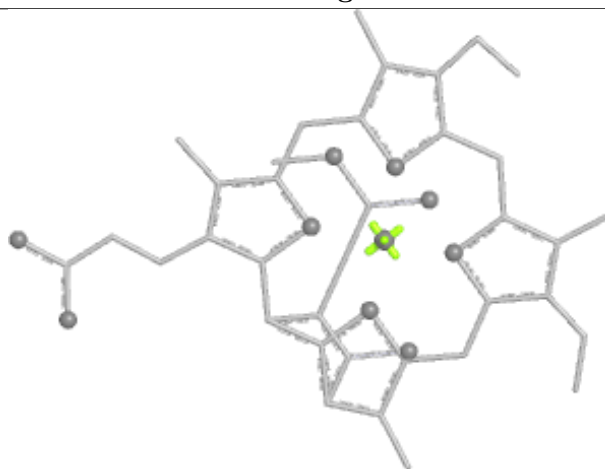
Bond lengths



Bond angles

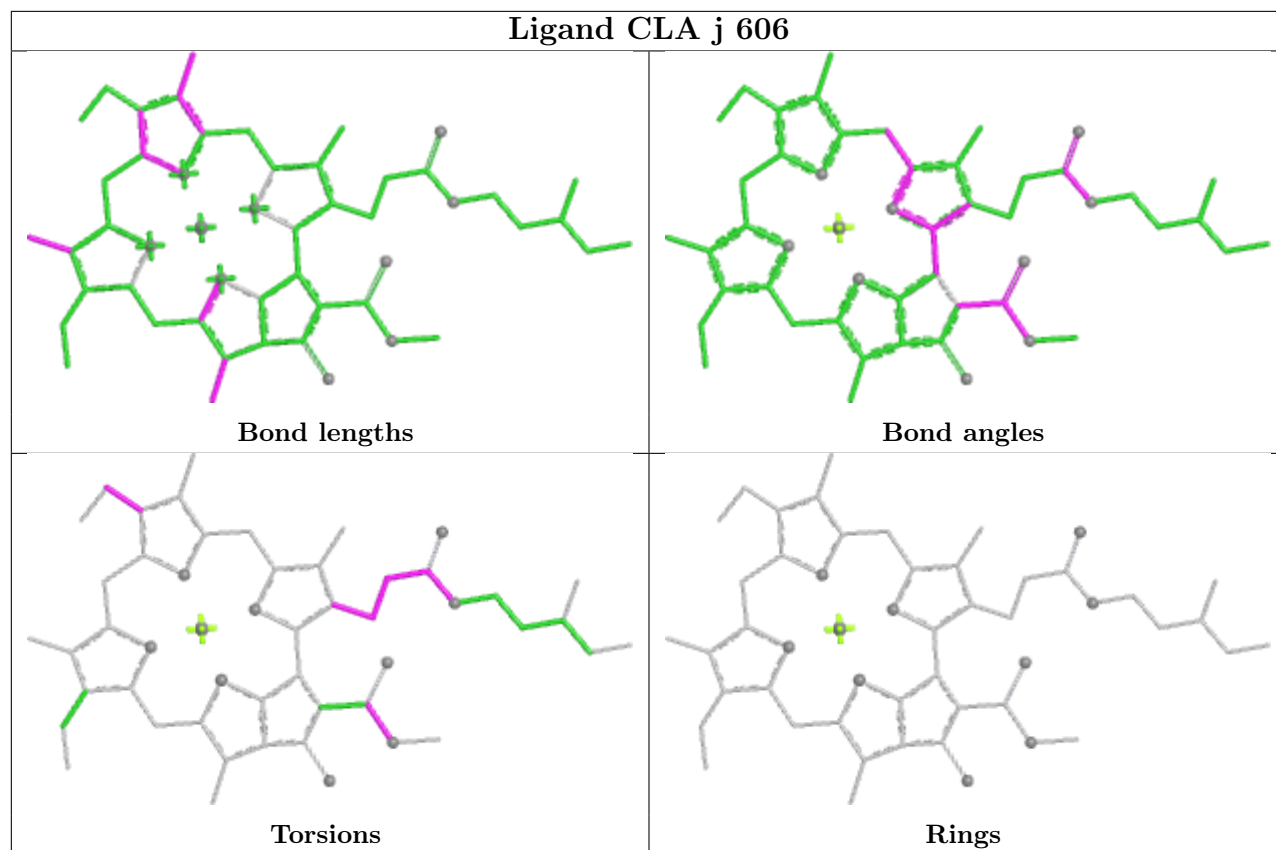


Torsions

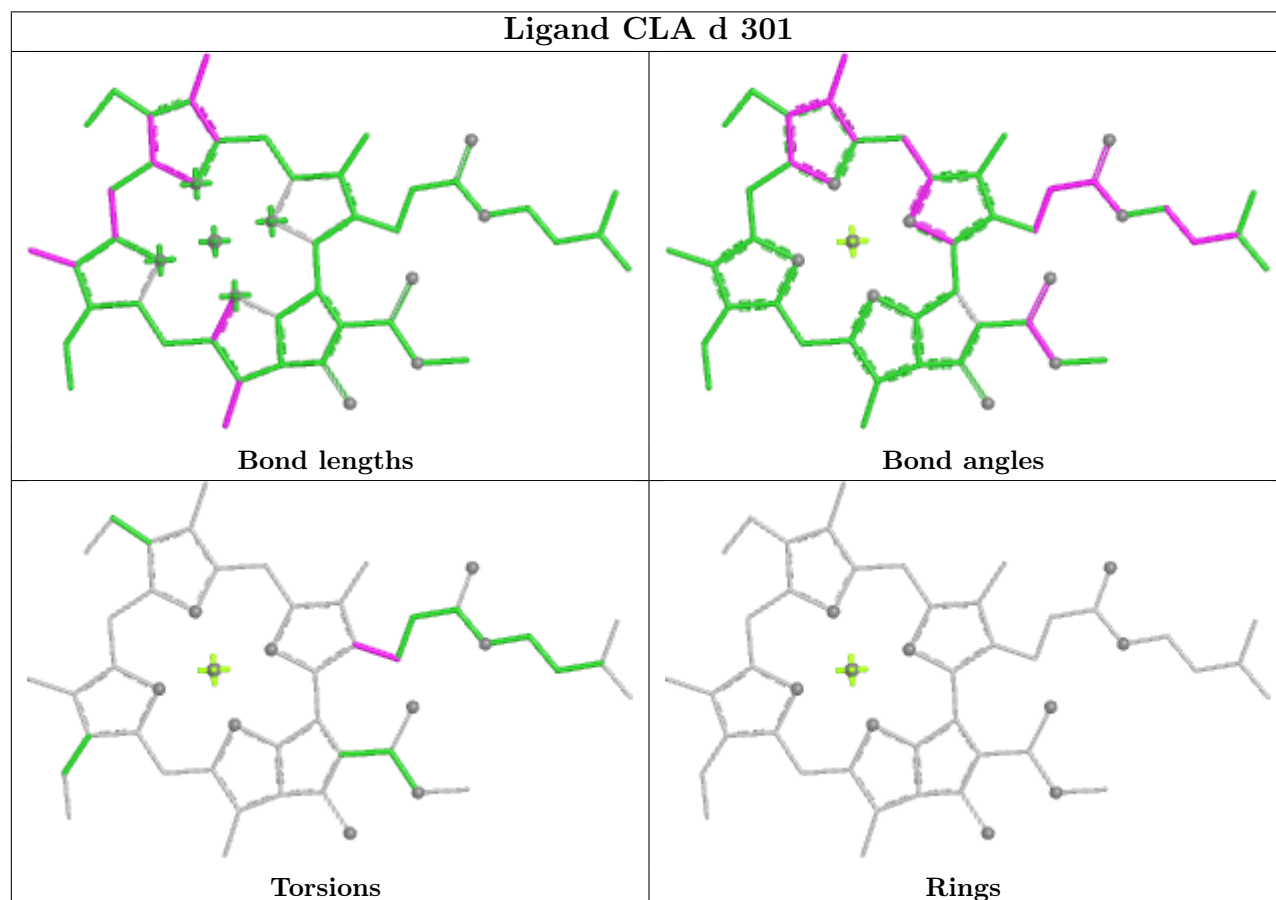


Rings

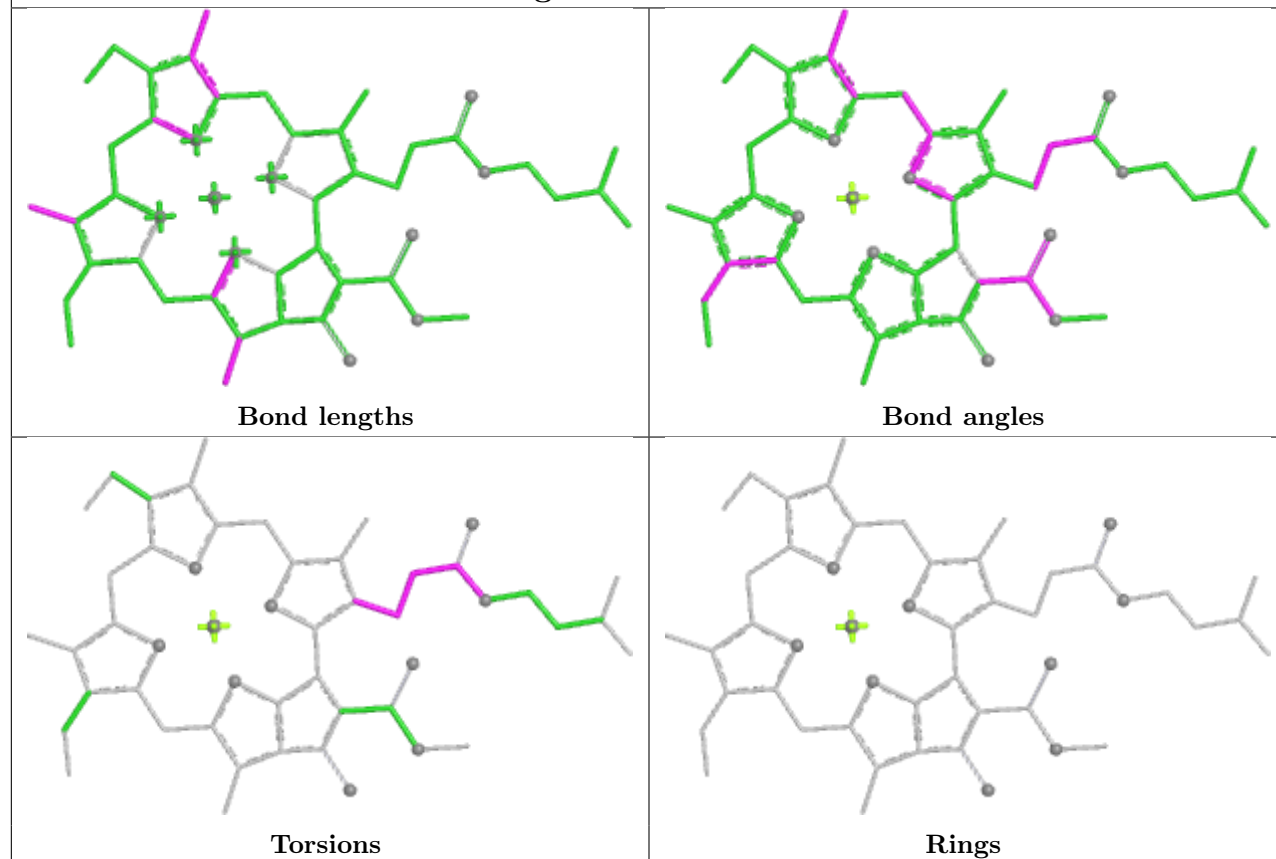
## Ligand CLA j 606



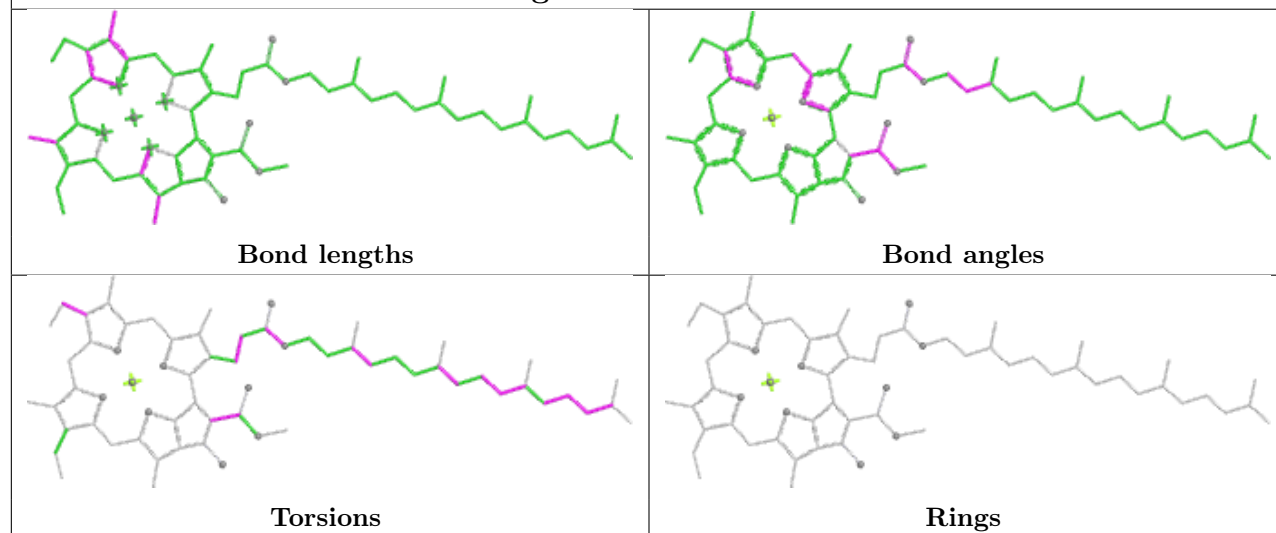
## Ligand CLA d 301

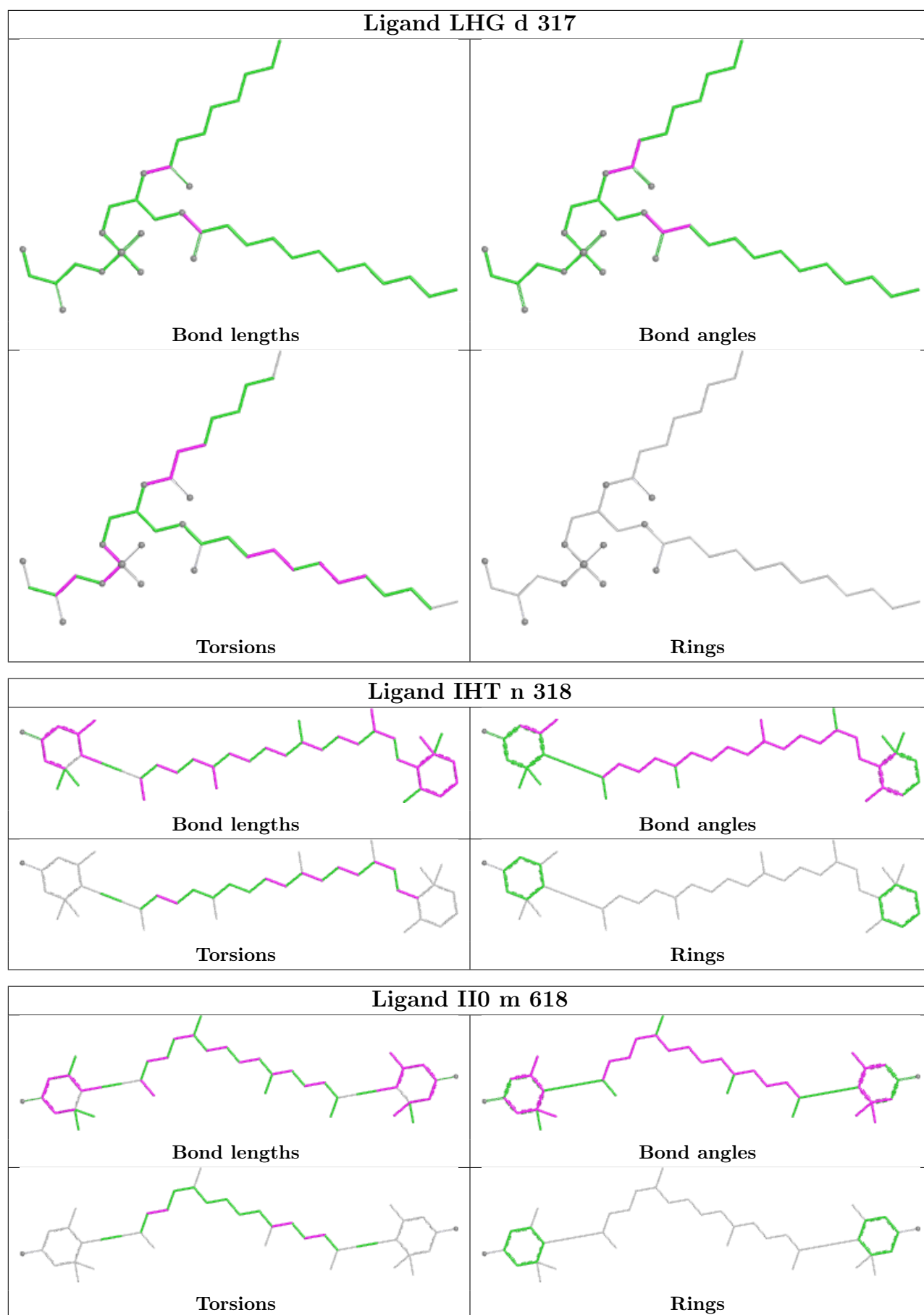


## Ligand CLA L 204



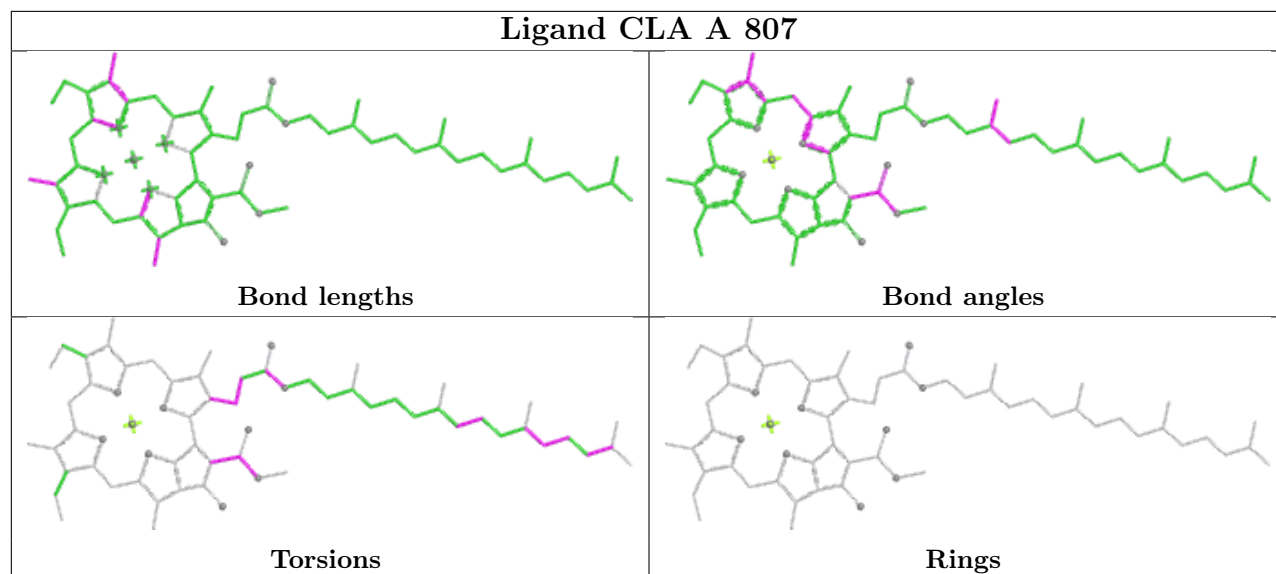
## Ligand CLA A 835



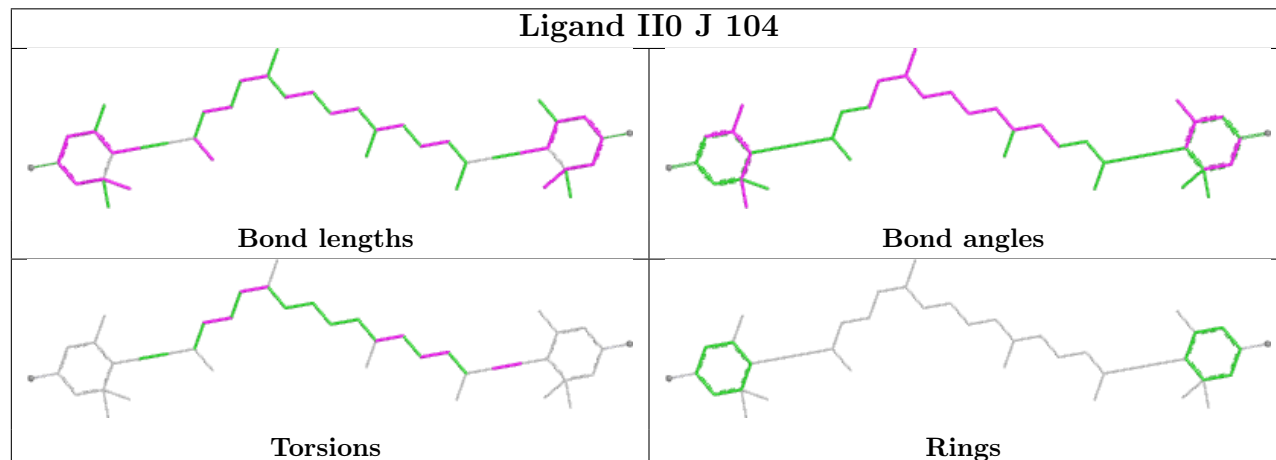




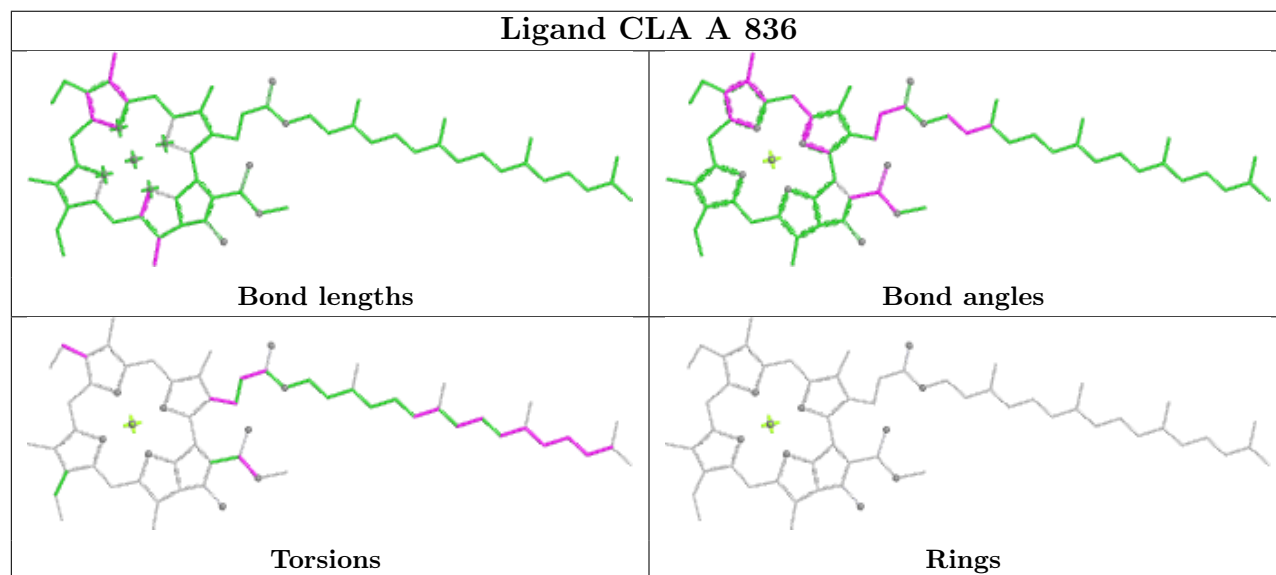
## Ligand CLA A 807

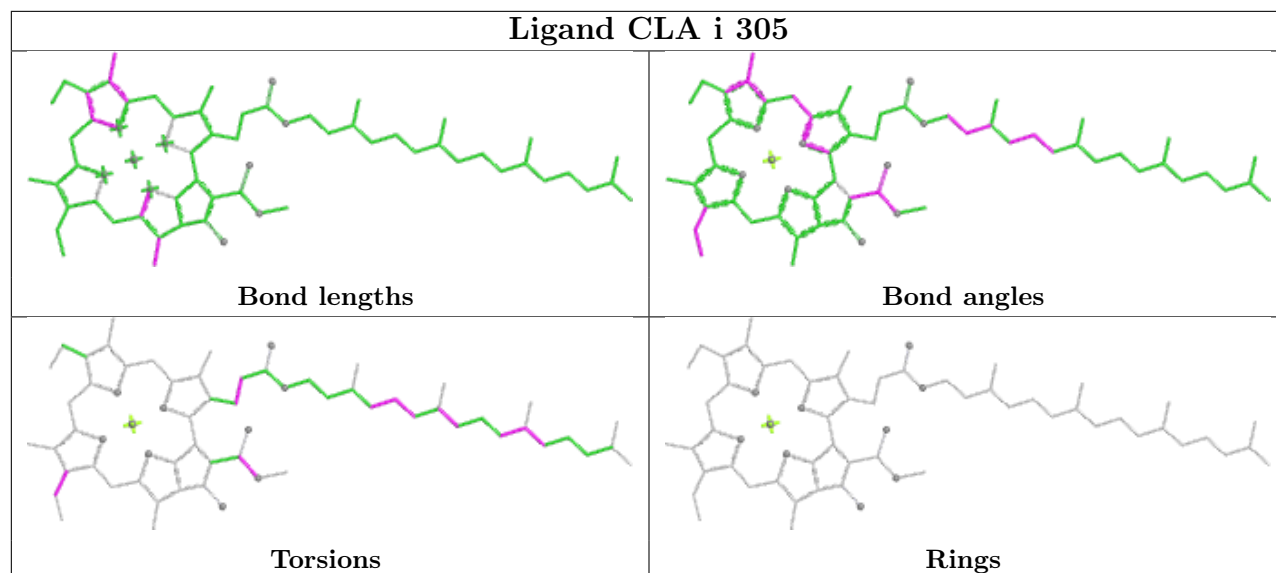
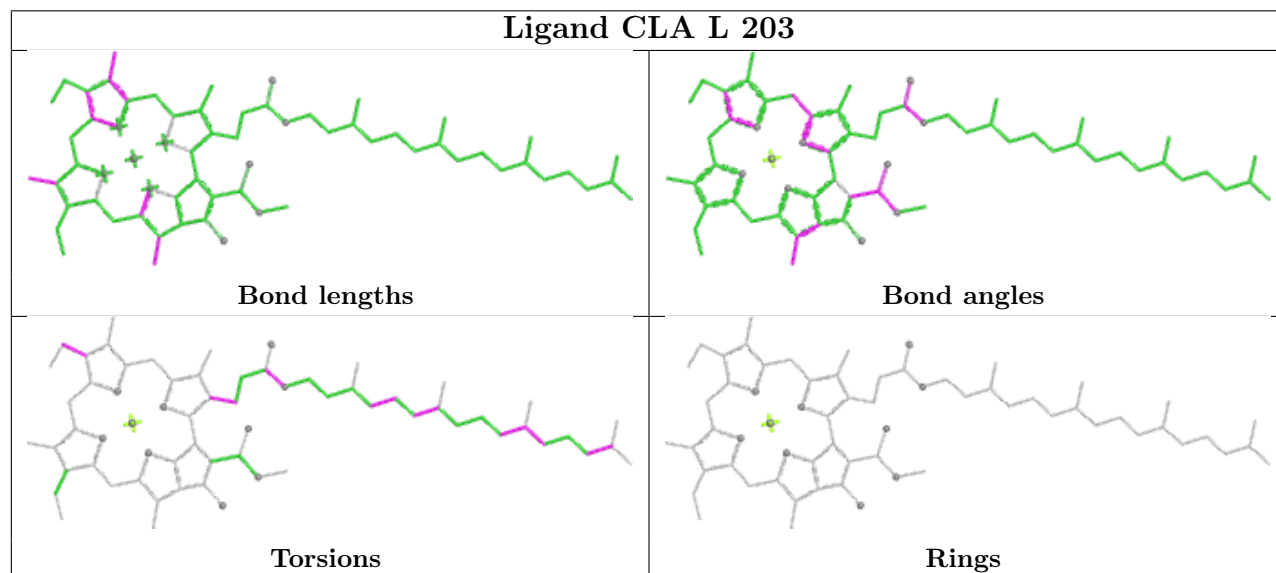
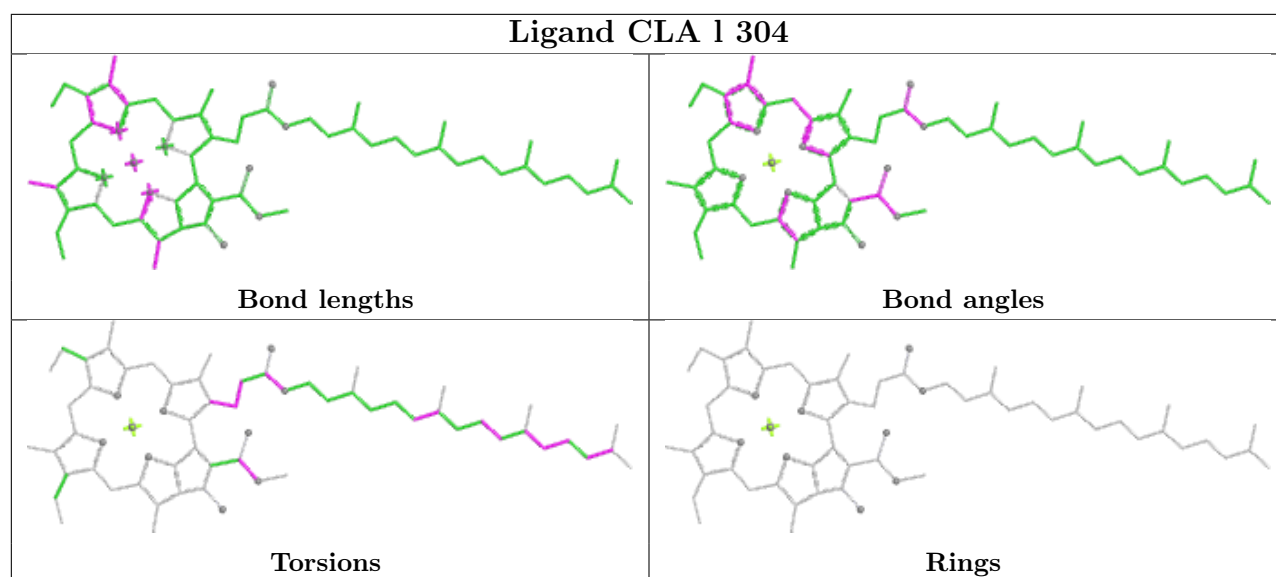


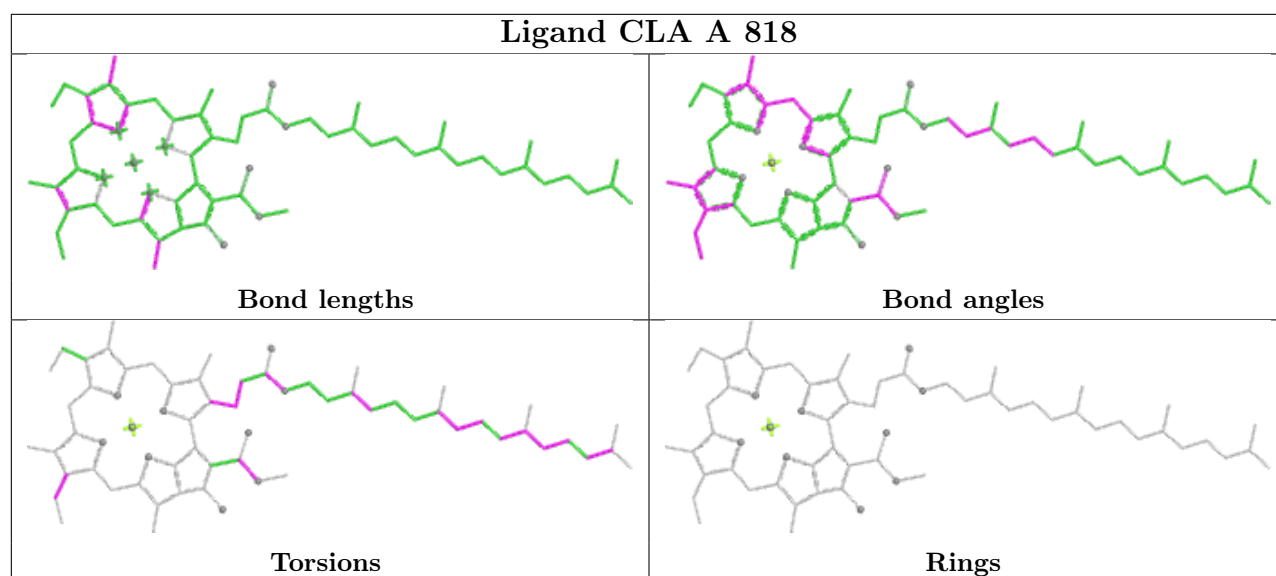
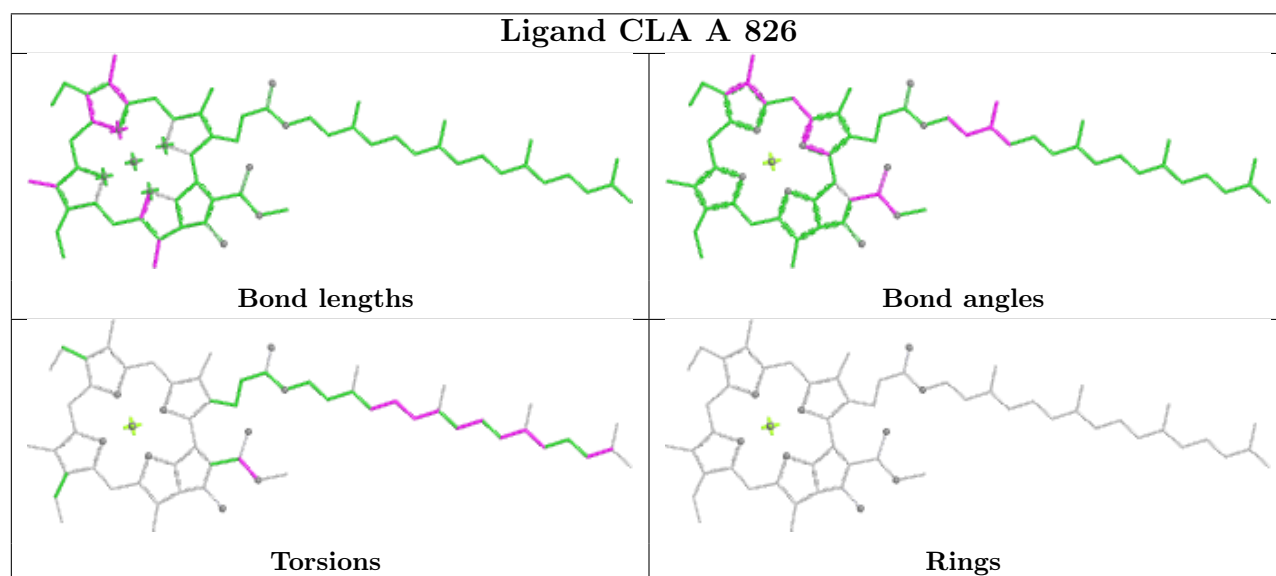
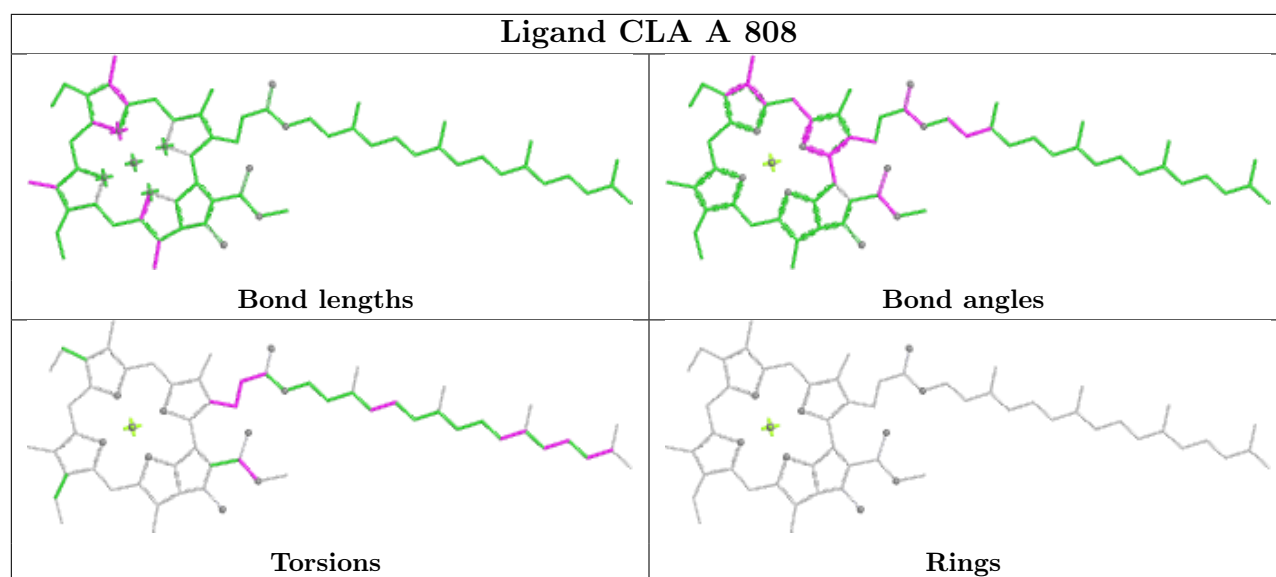
## Ligand II0 J 104



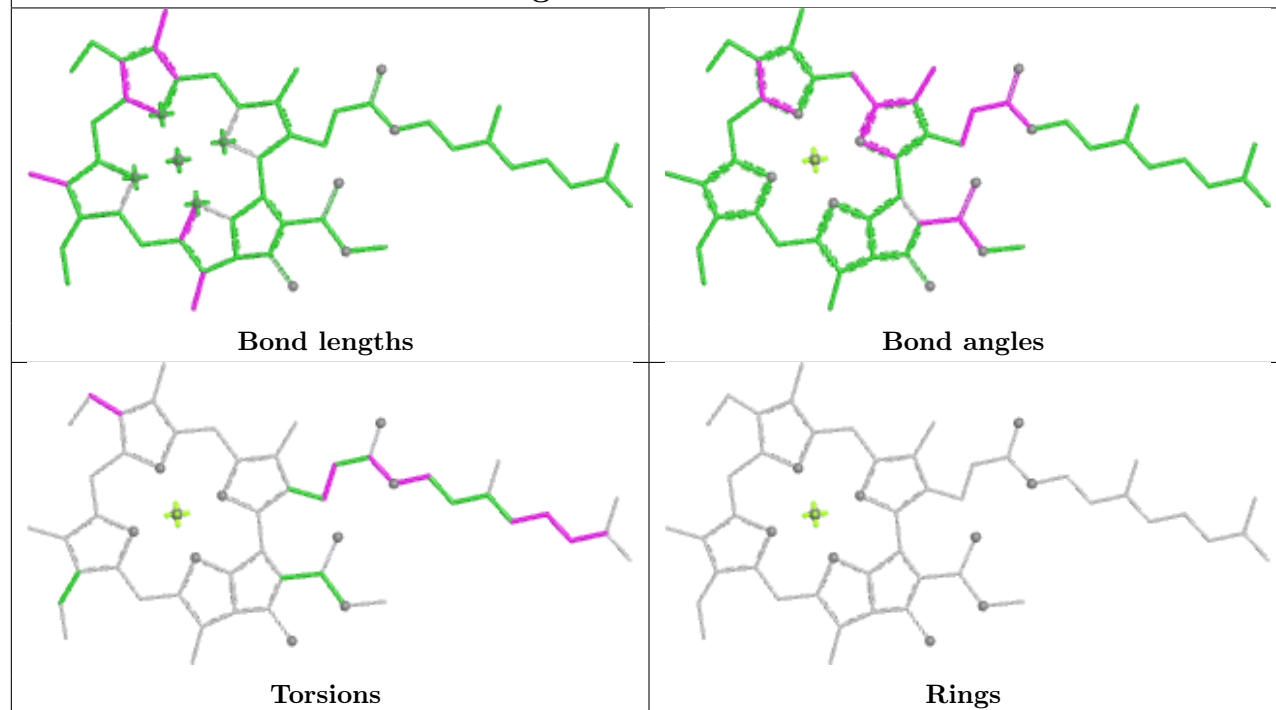
## Ligand CLA A 836



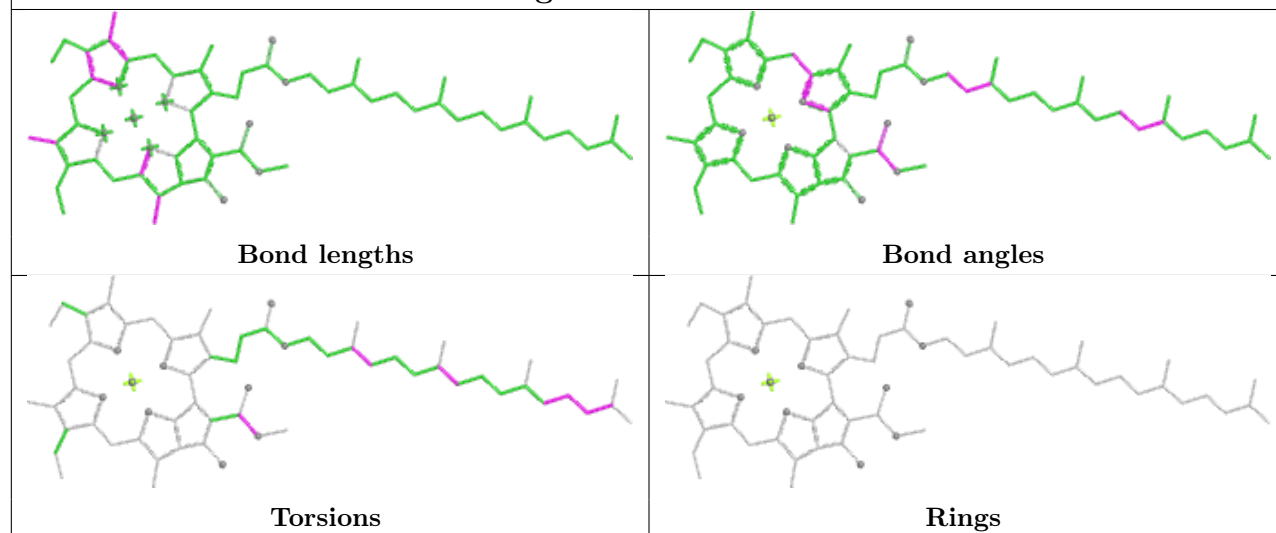




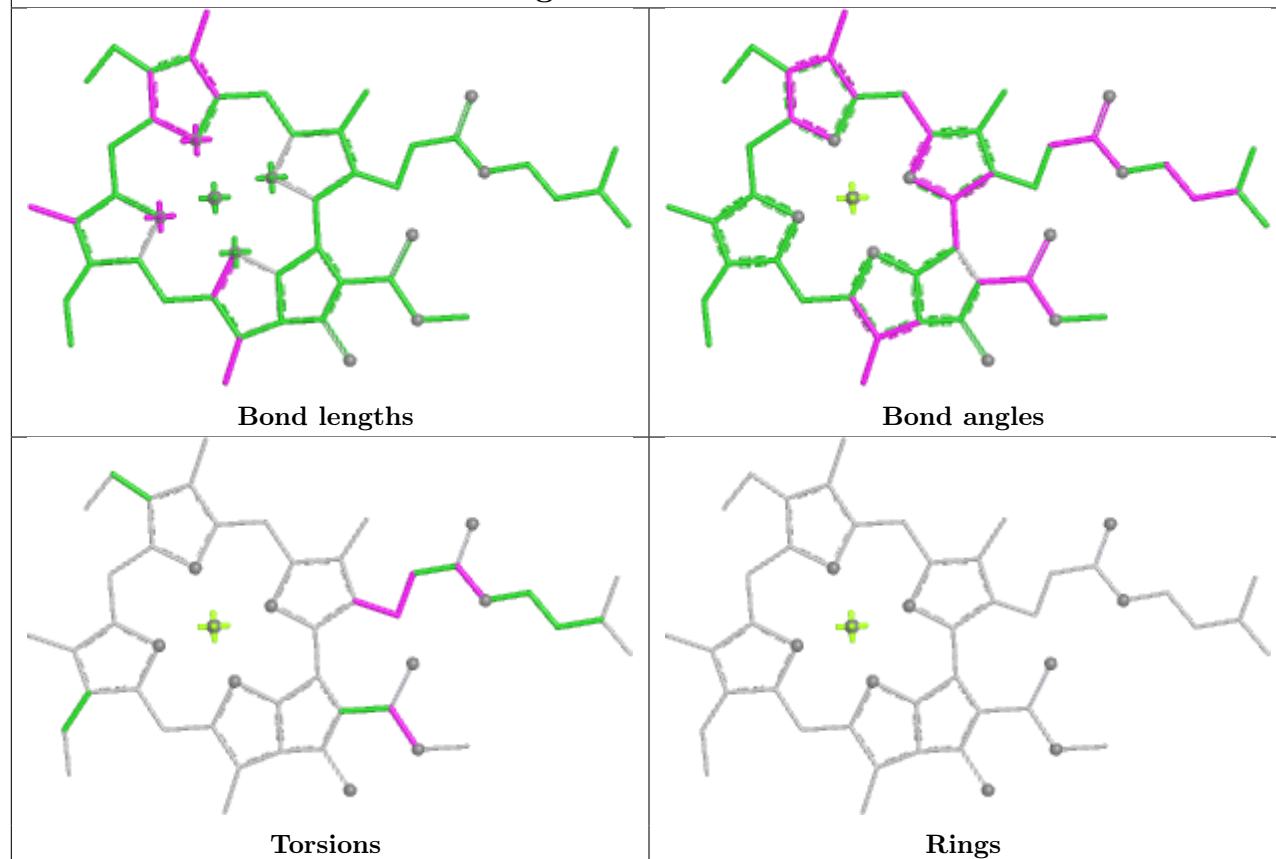
## Ligand CLA B 811



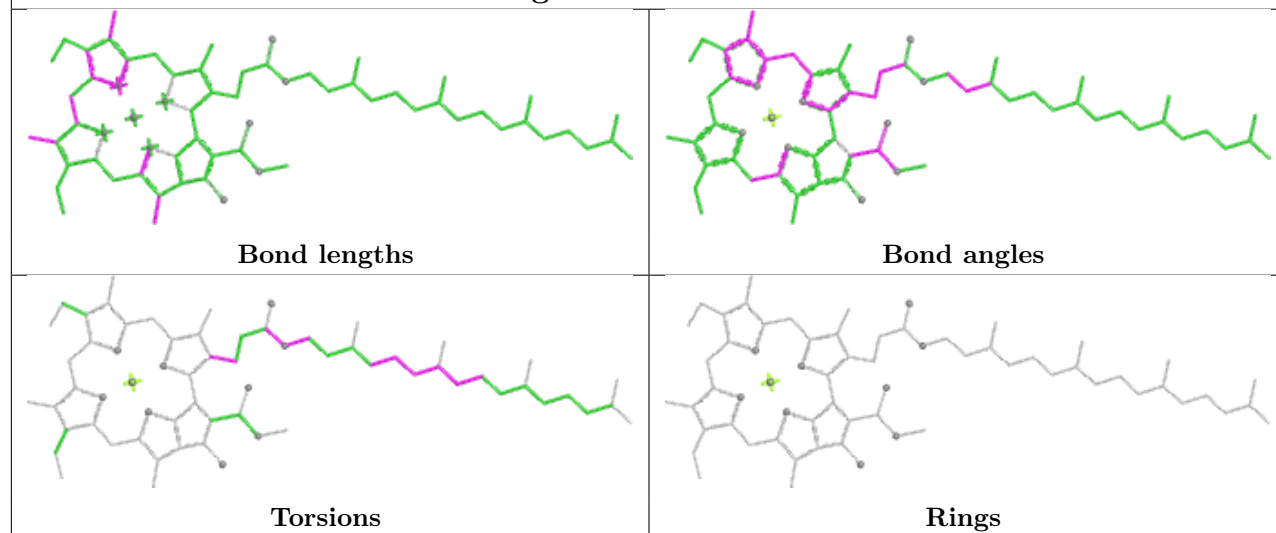
## Ligand CLA b 608

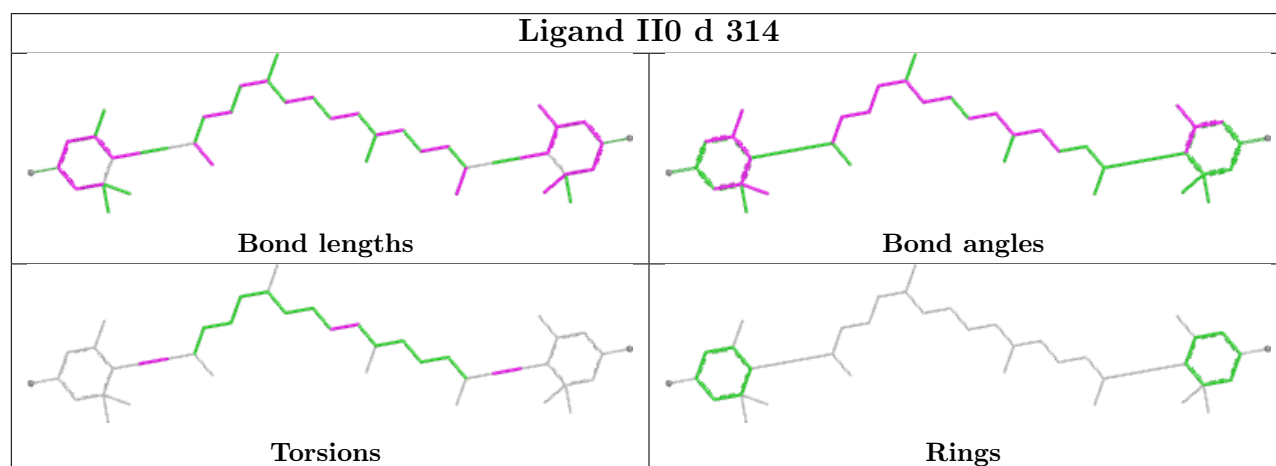
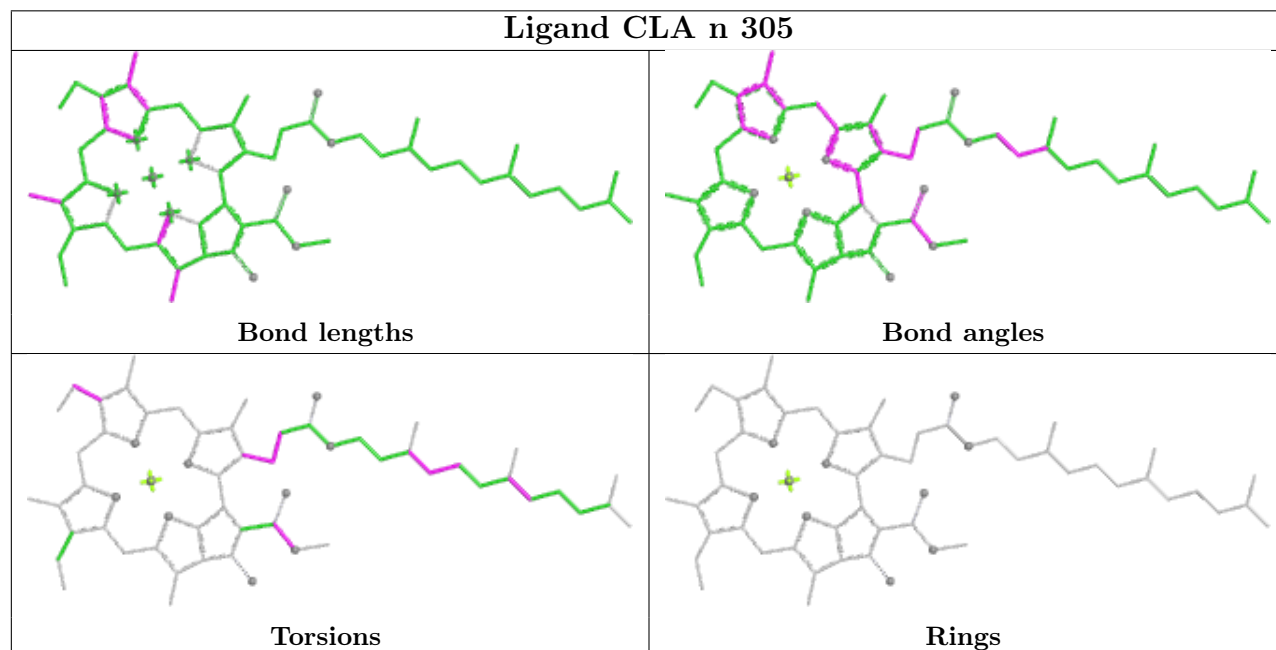
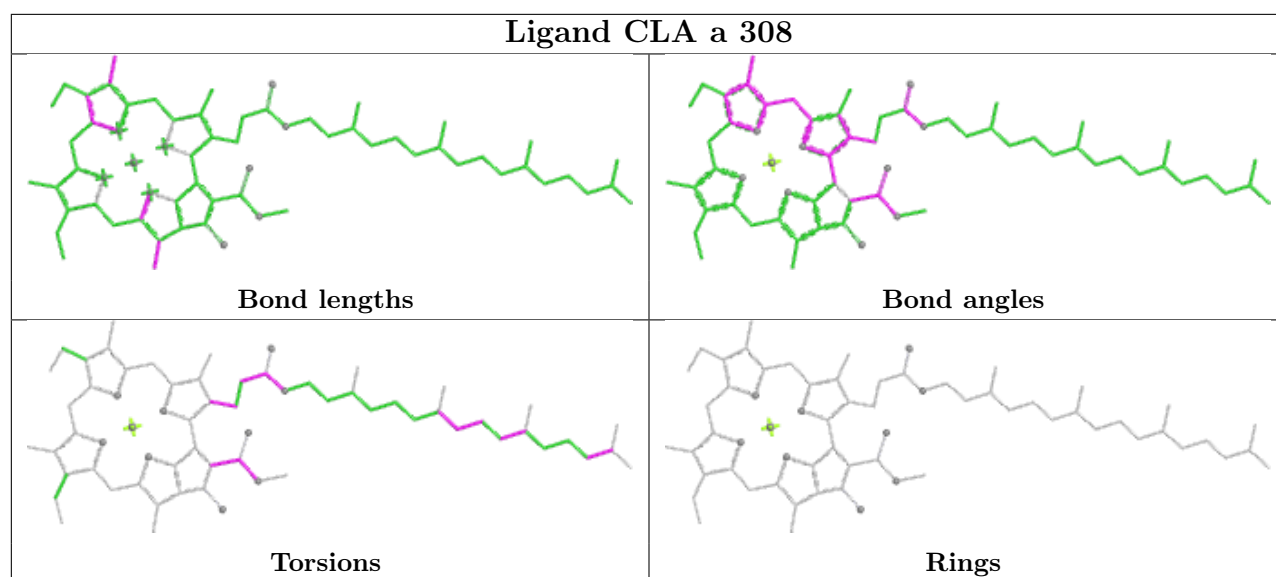


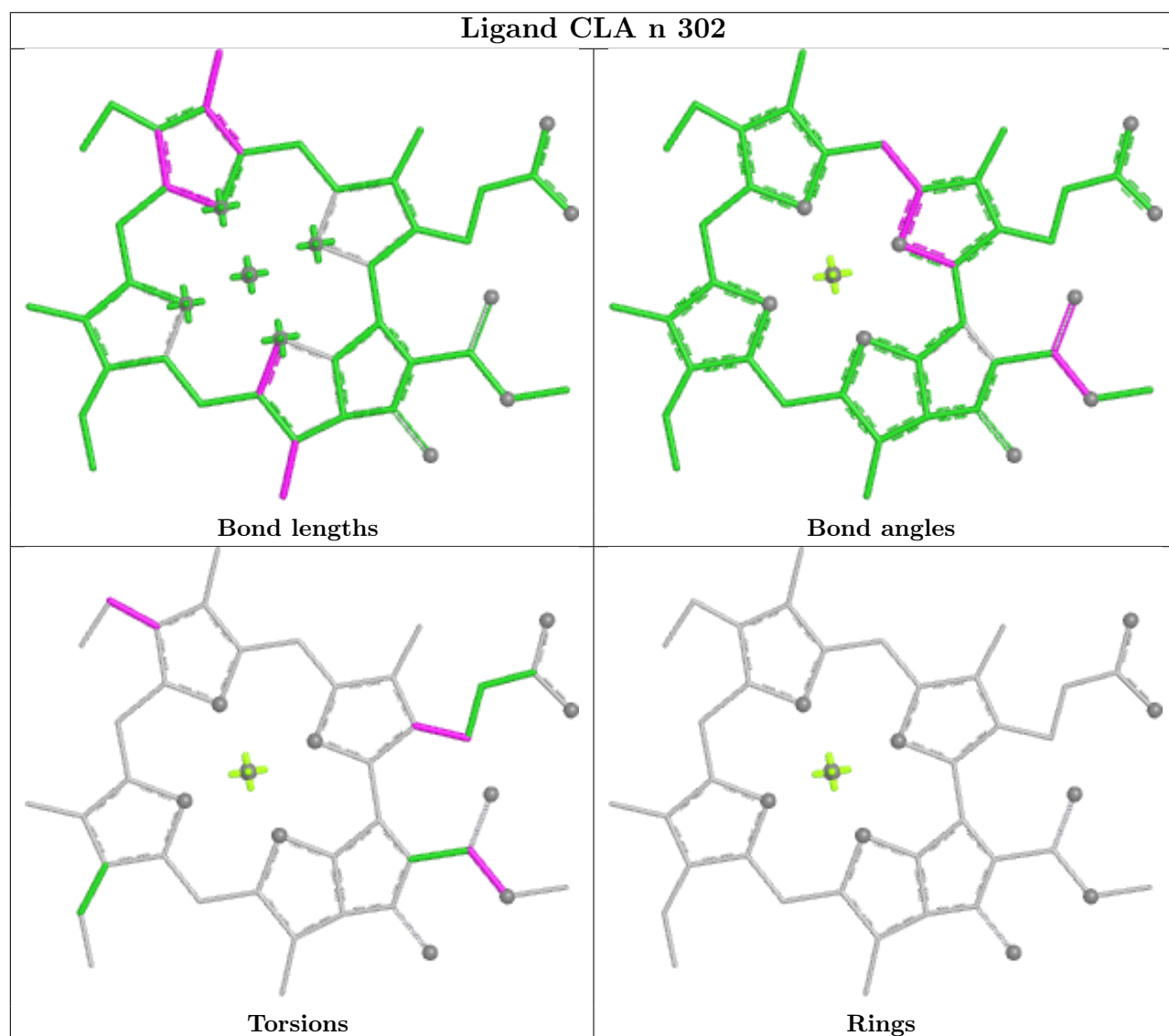
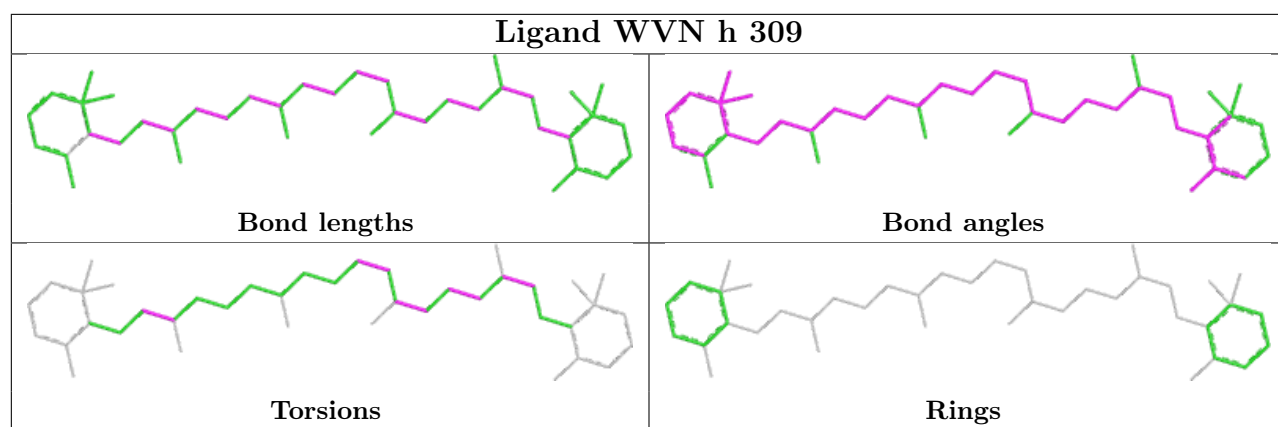
## Ligand CLA k 602



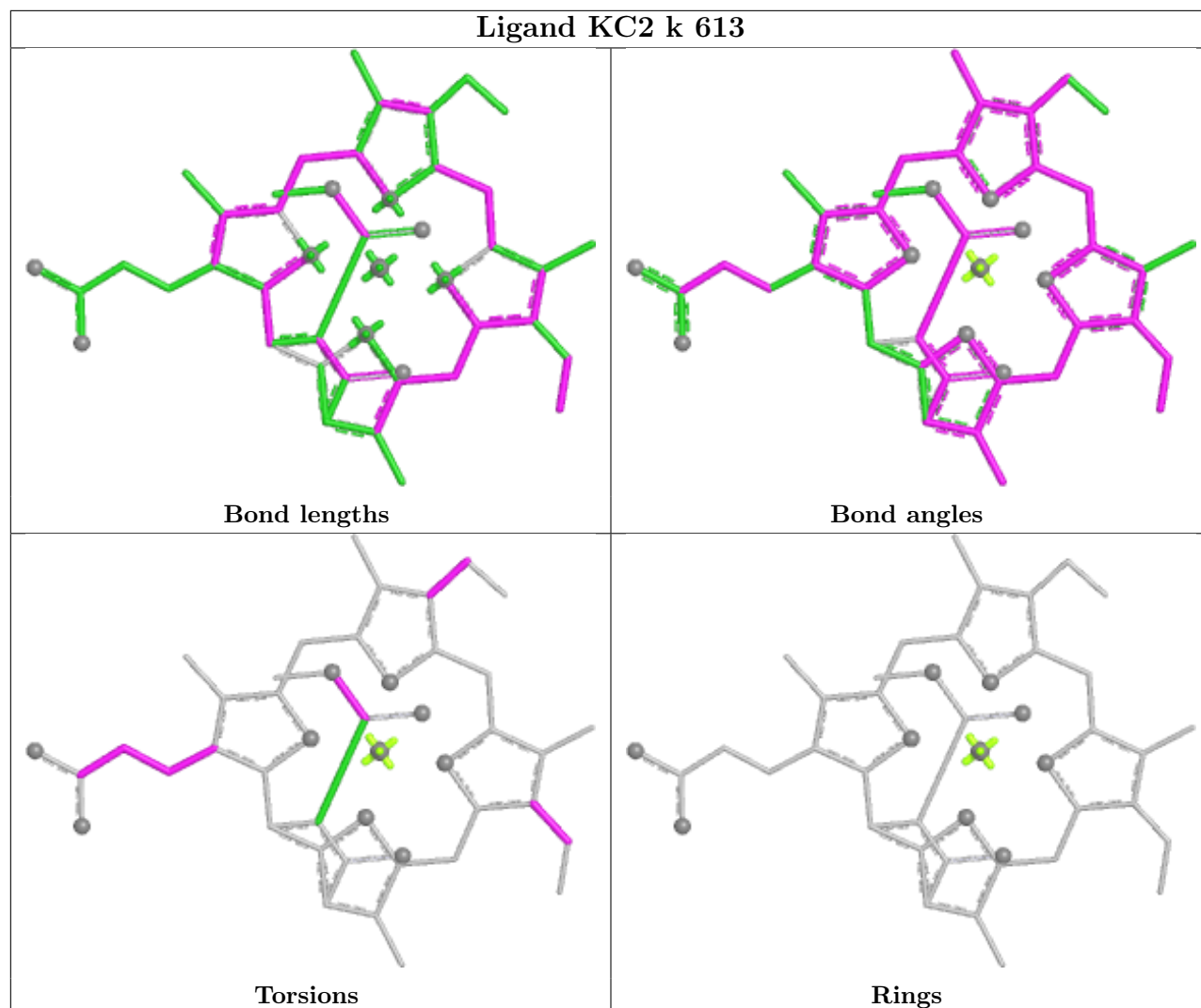
## Ligand CLA A 802



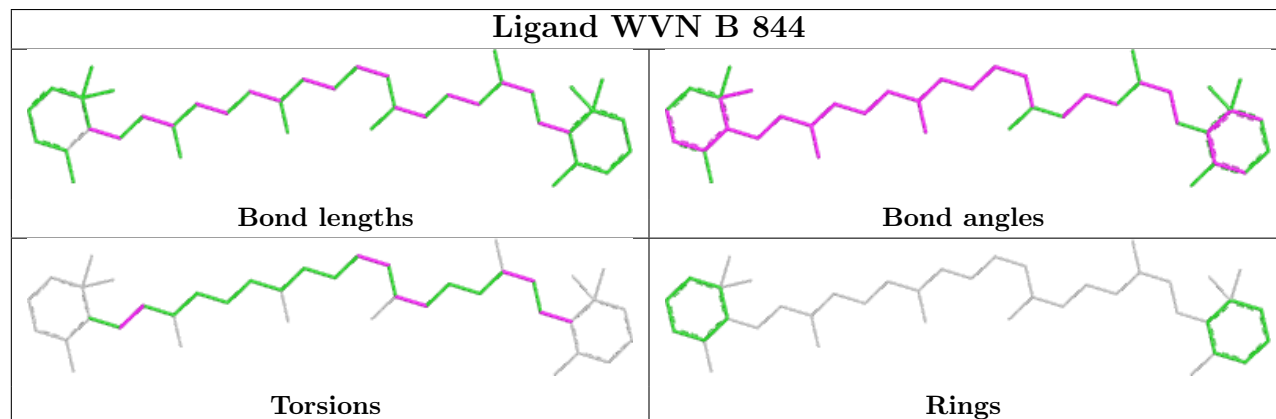




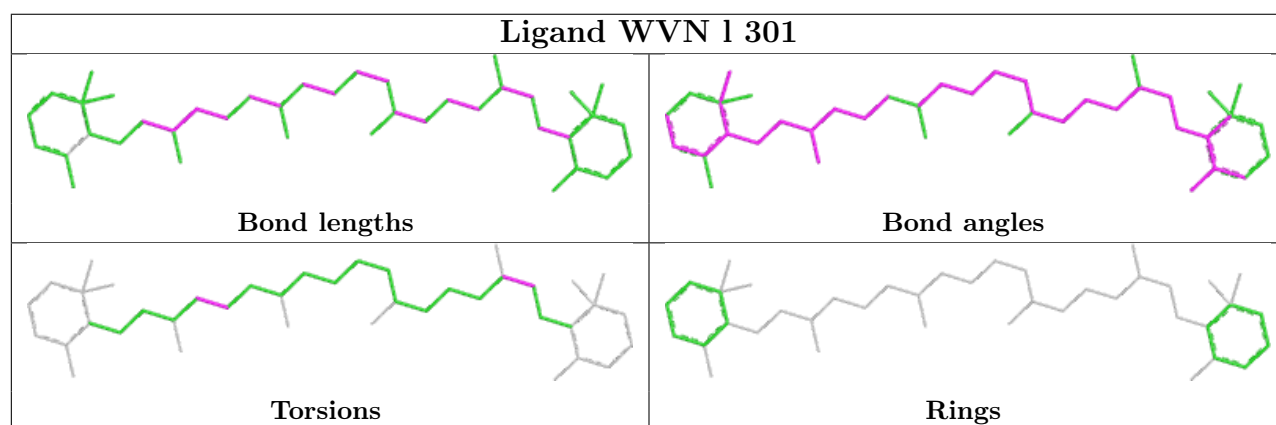
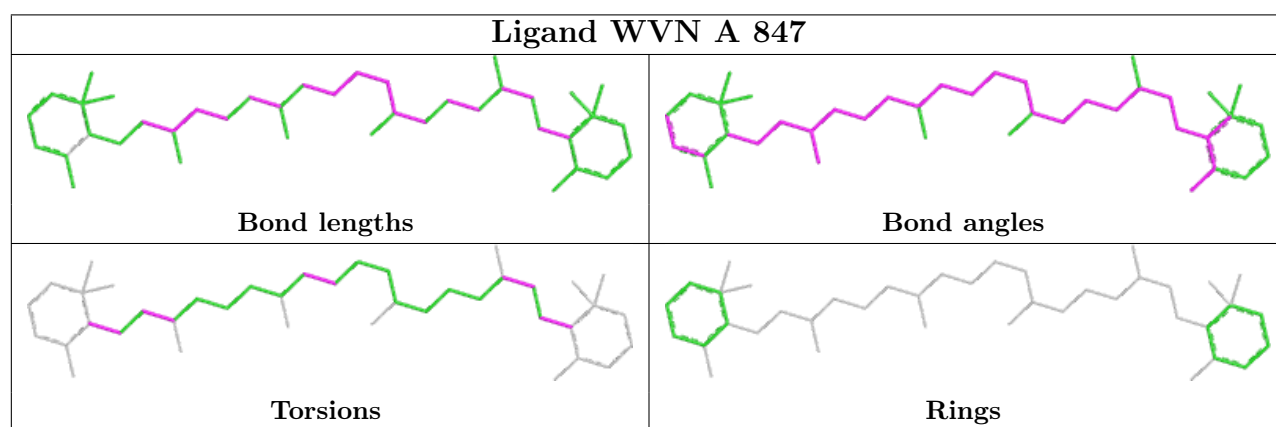
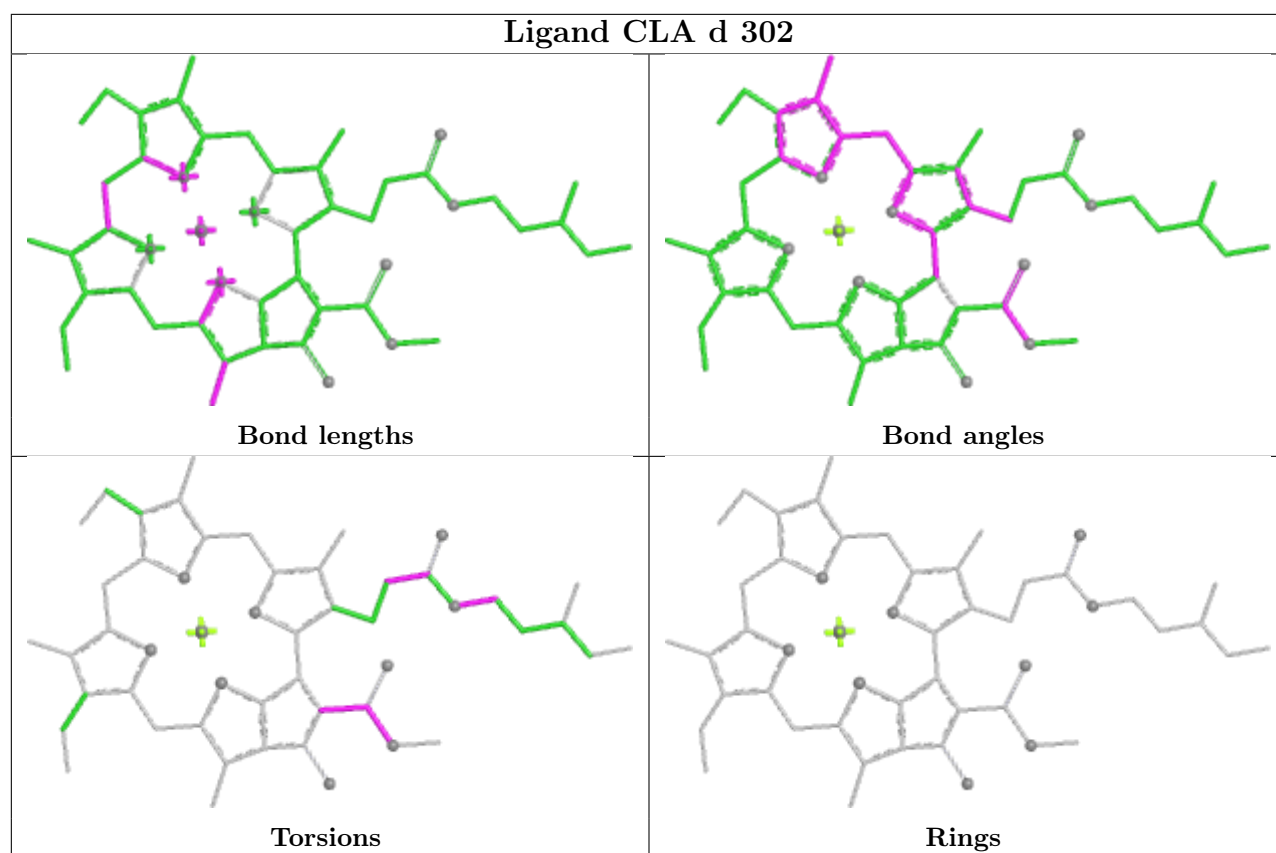
## Ligand KC2 k 613

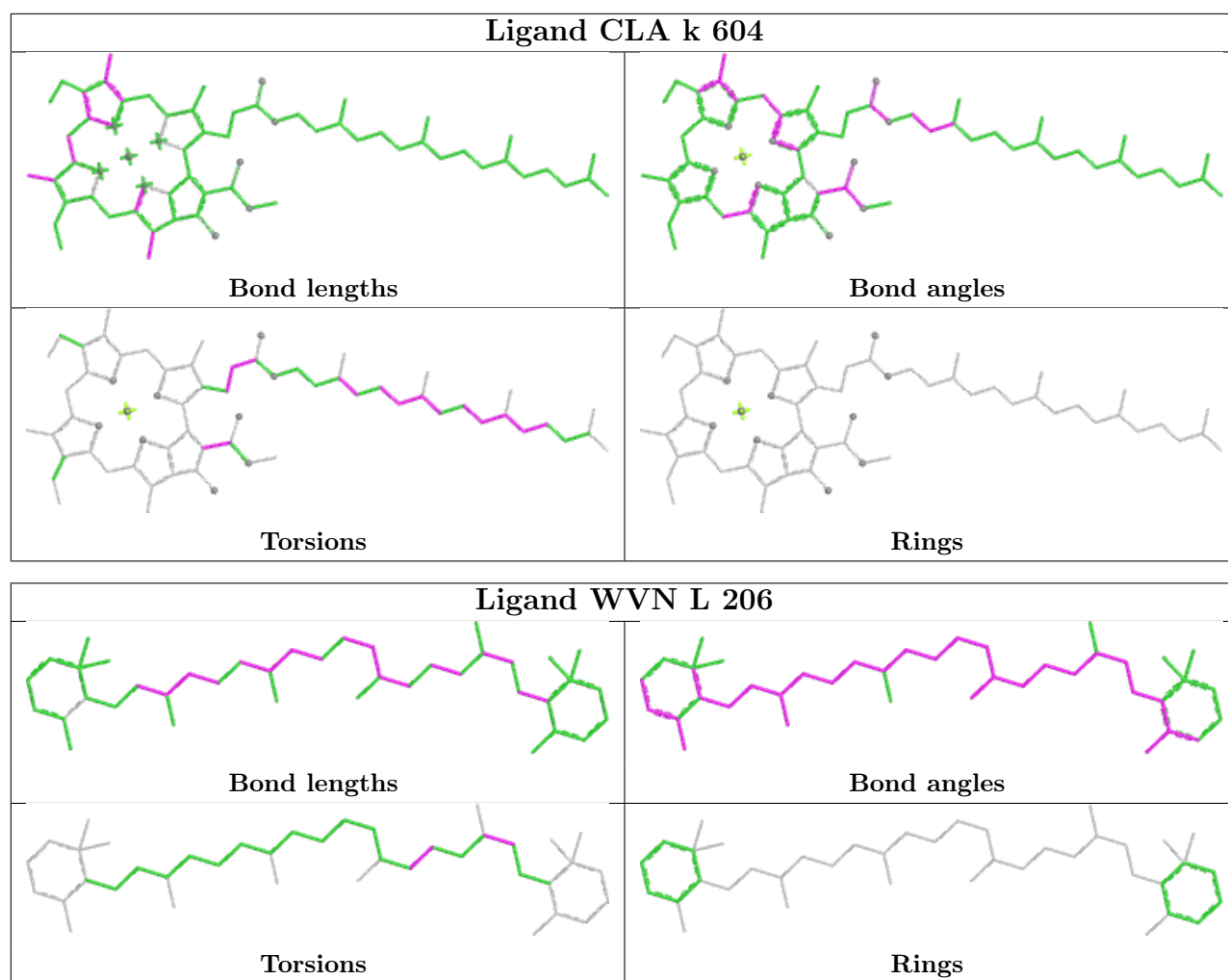


## Ligand WVN B 844

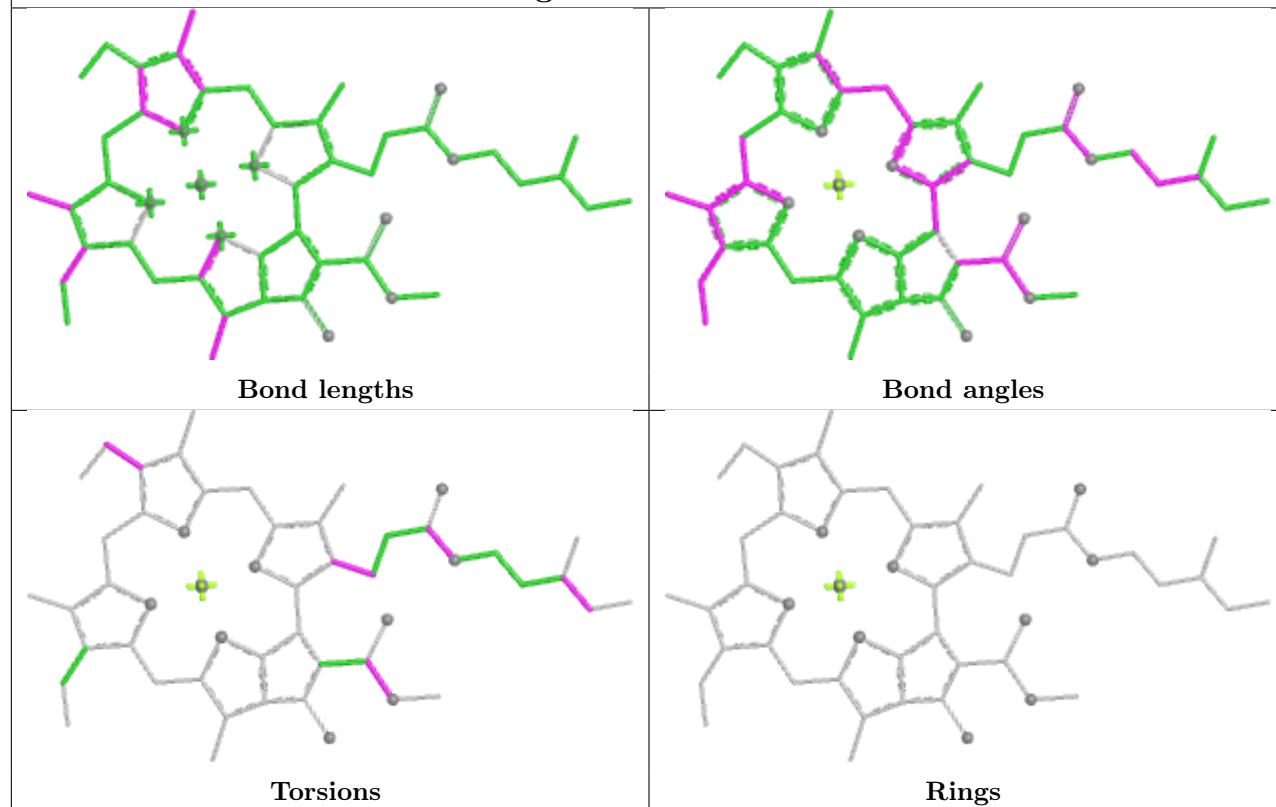




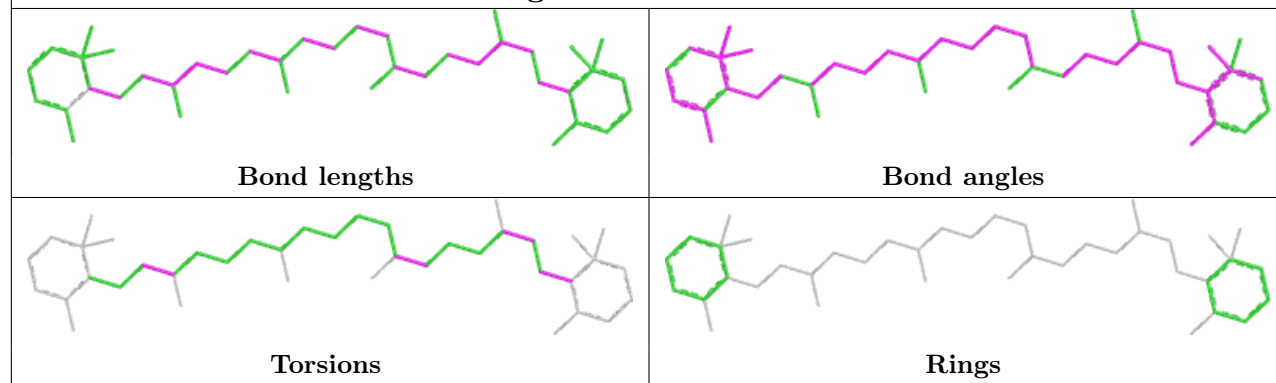


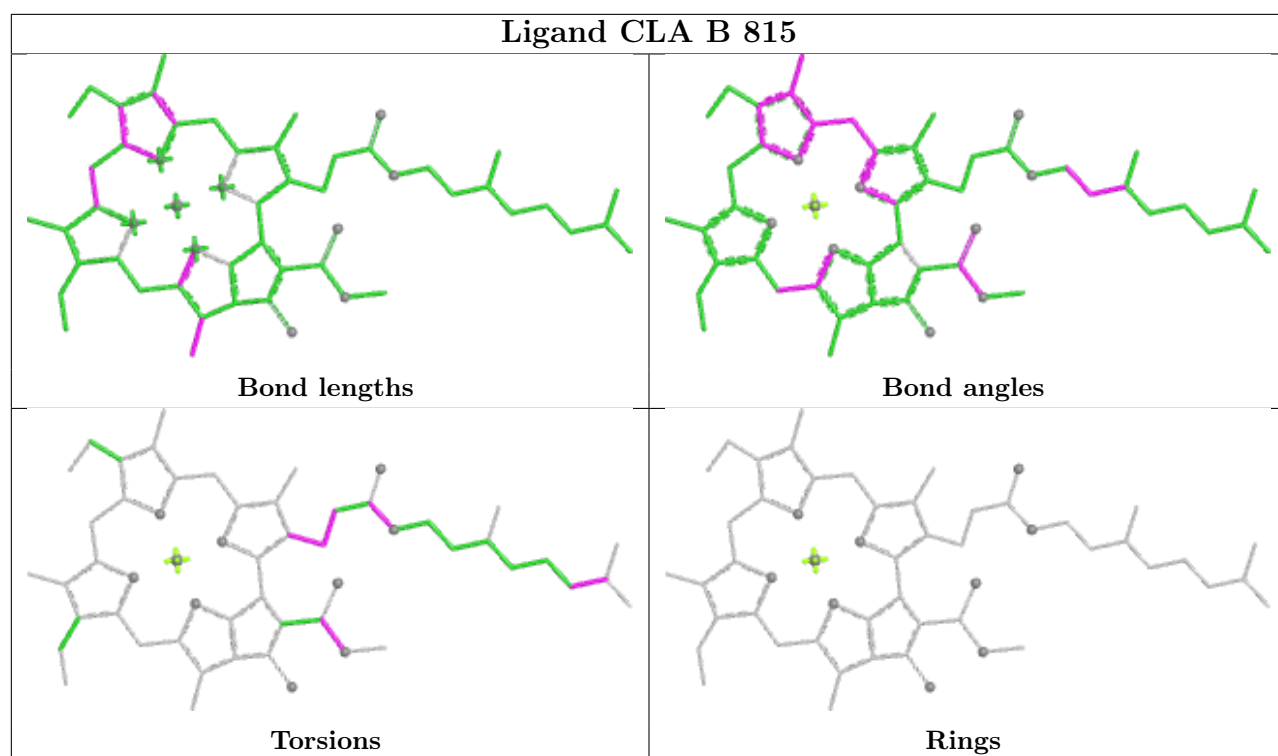


## Ligand CLA n 304

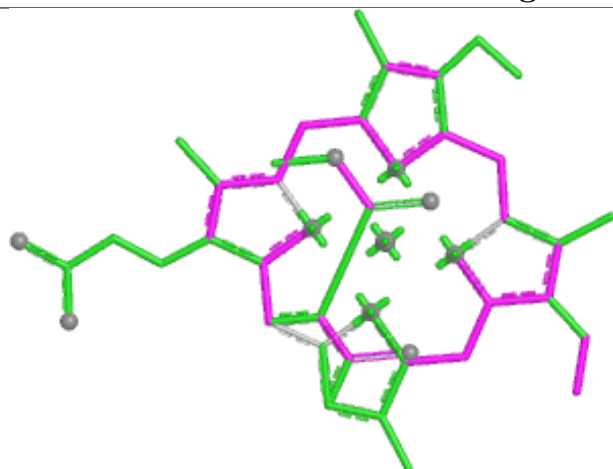


## Ligand WVN J 102

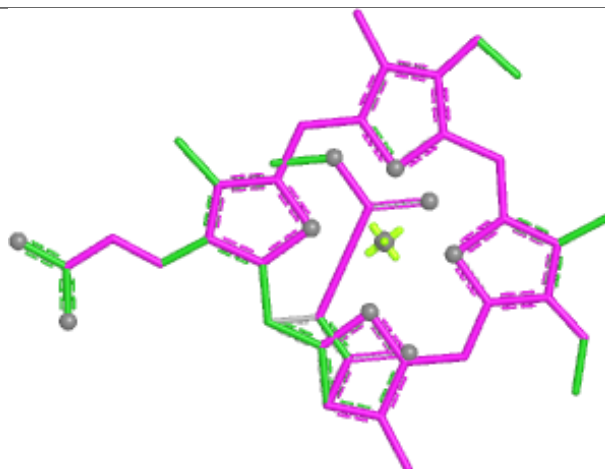




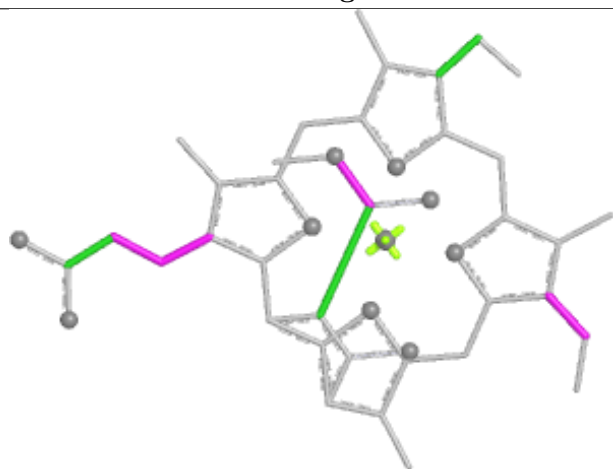
## Ligand KC2 d 311



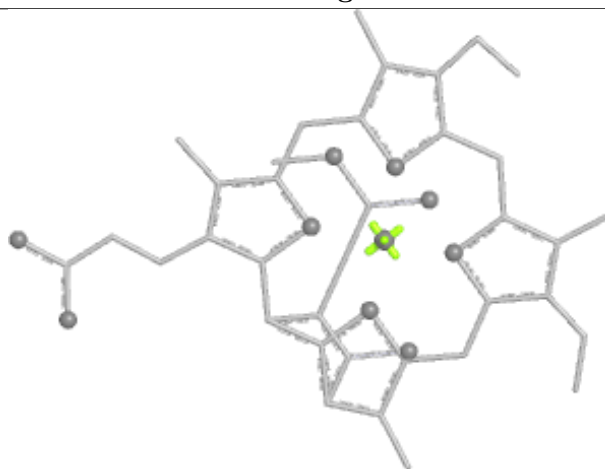
Bond lengths



Bond angles

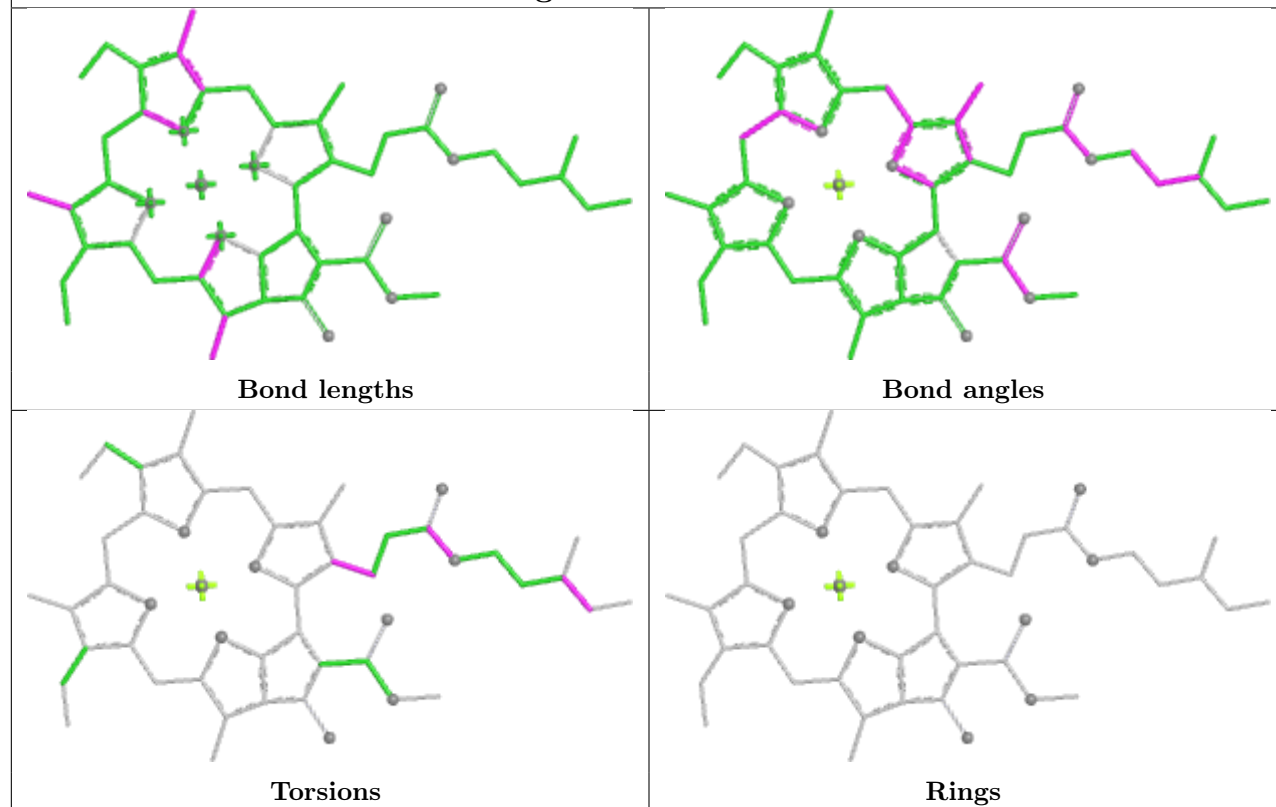


Torsions

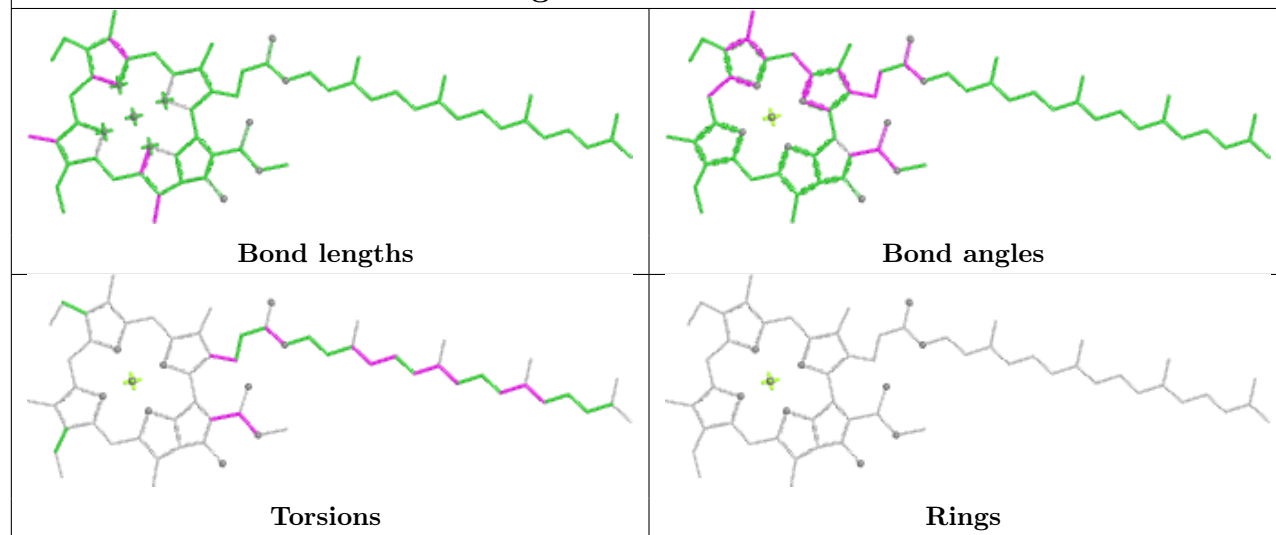


Rings

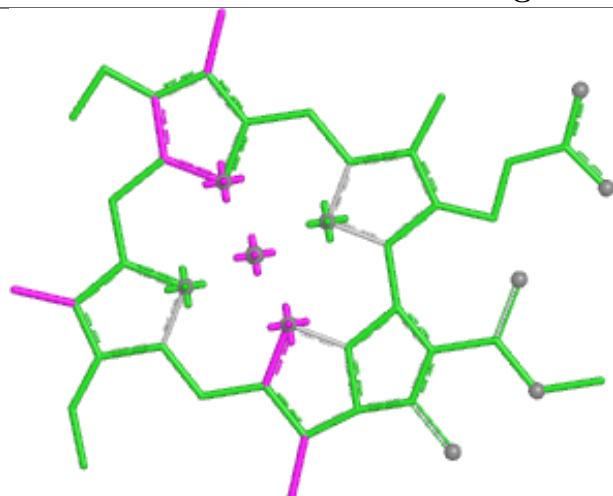
## Ligand CLA h 305



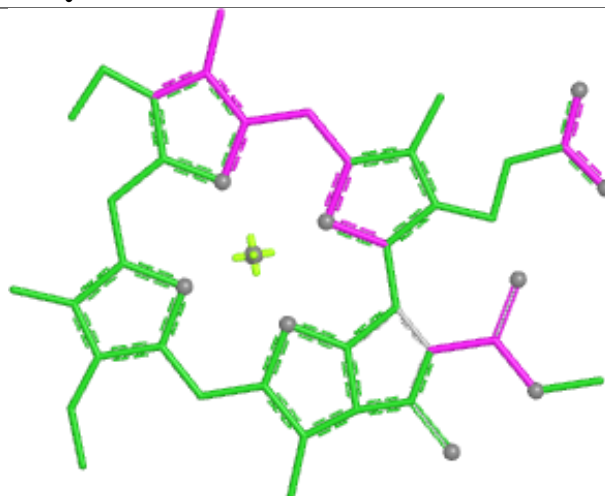
## Ligand CLA A 816



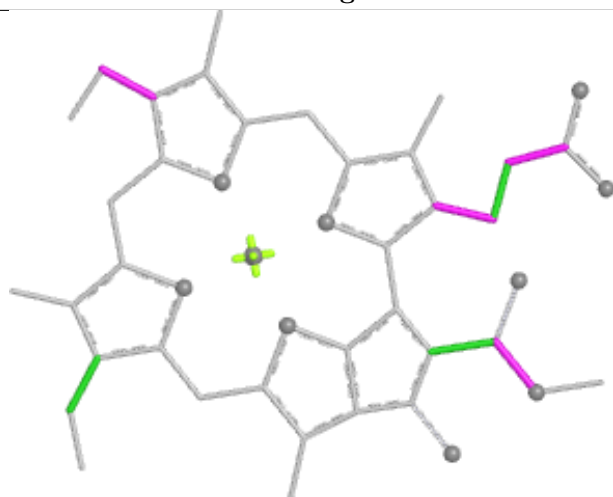
## Ligand CLA Q 303



Bond lengths



Bond angles

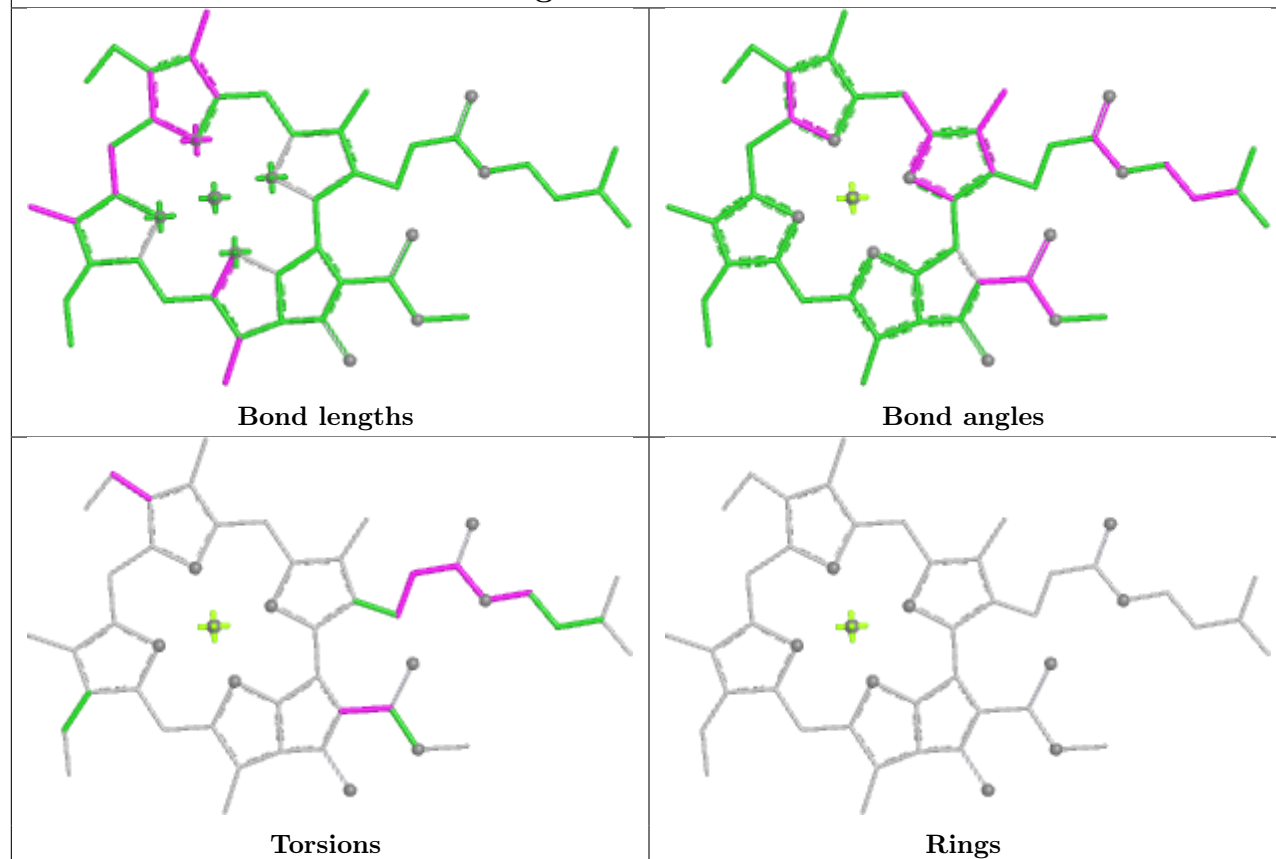


Torsions

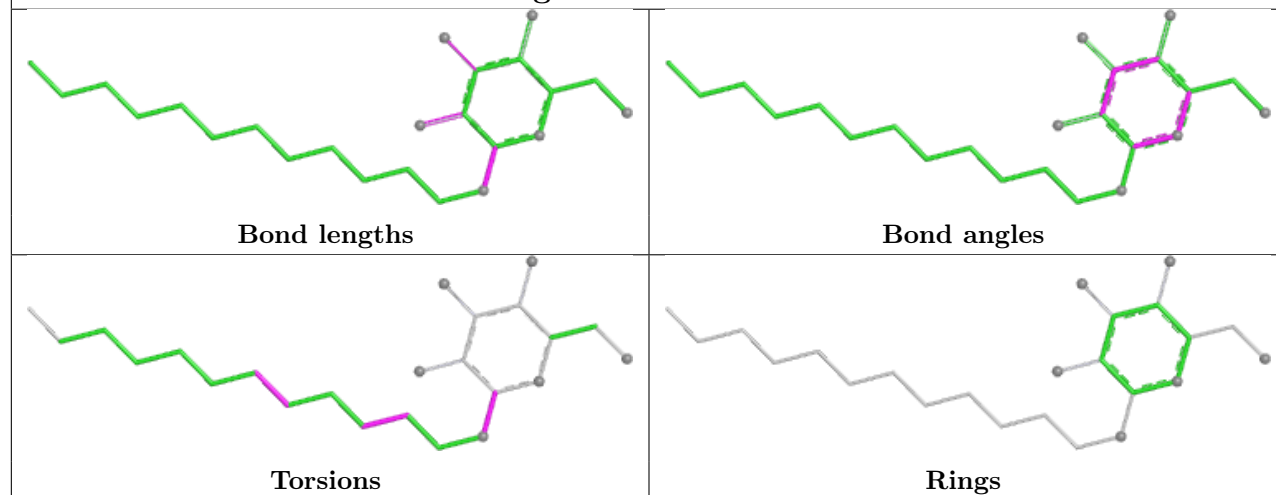


Rings

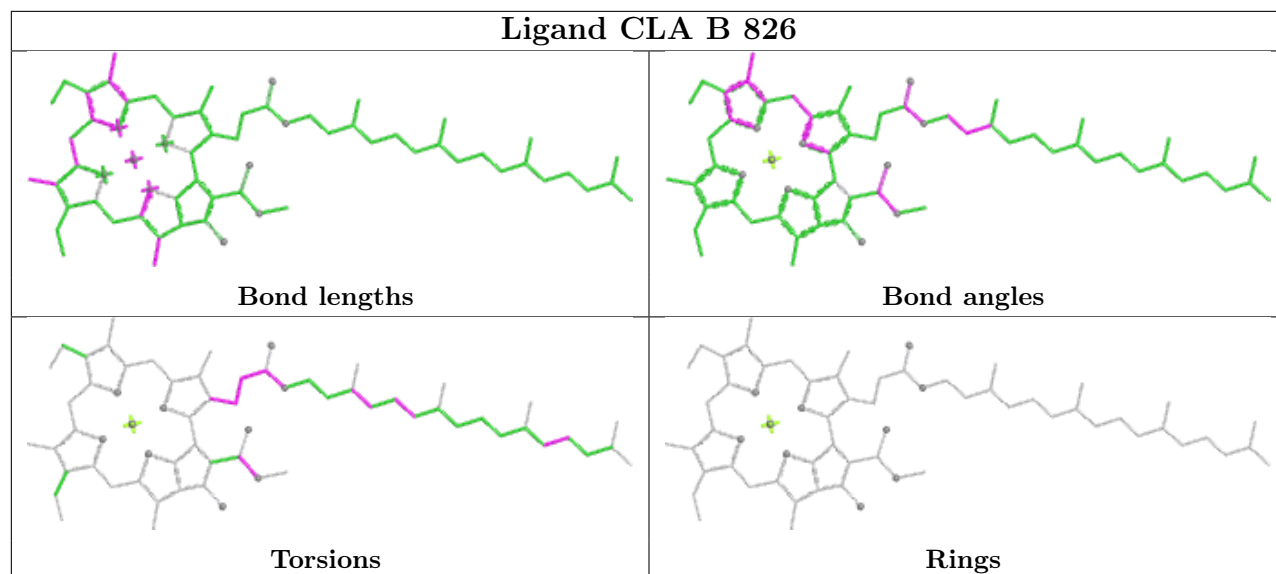
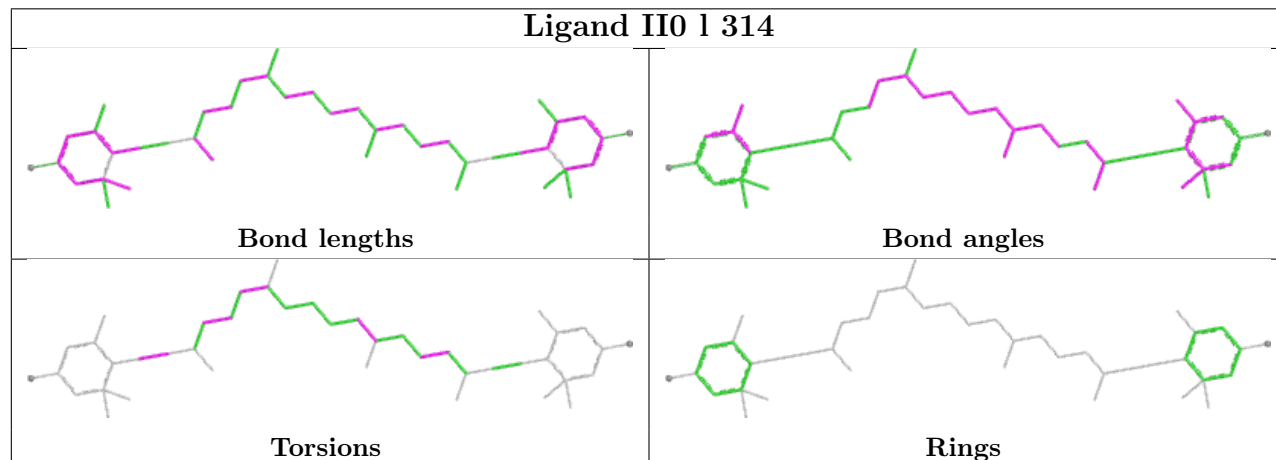
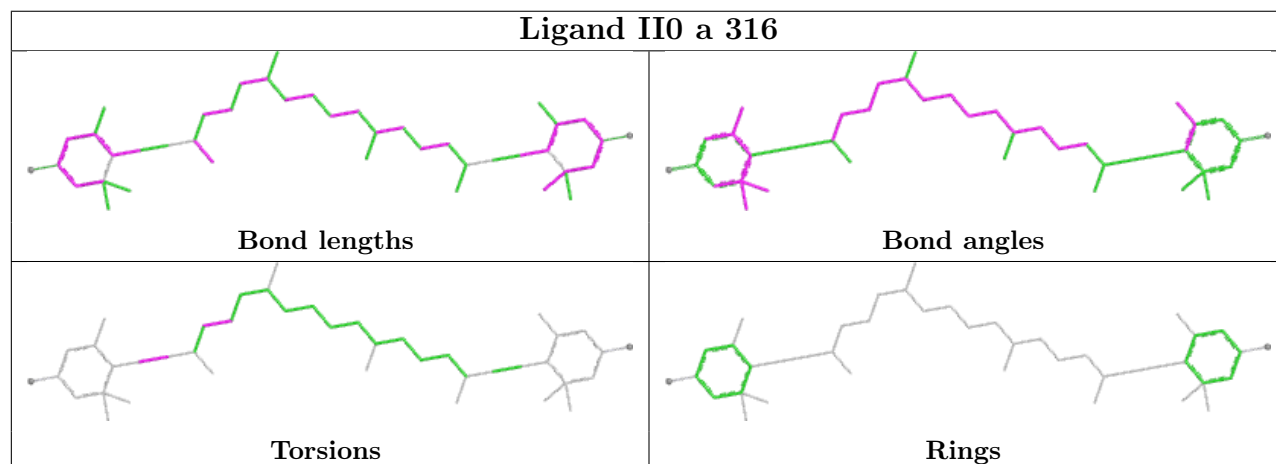
## Ligand CLA h 303



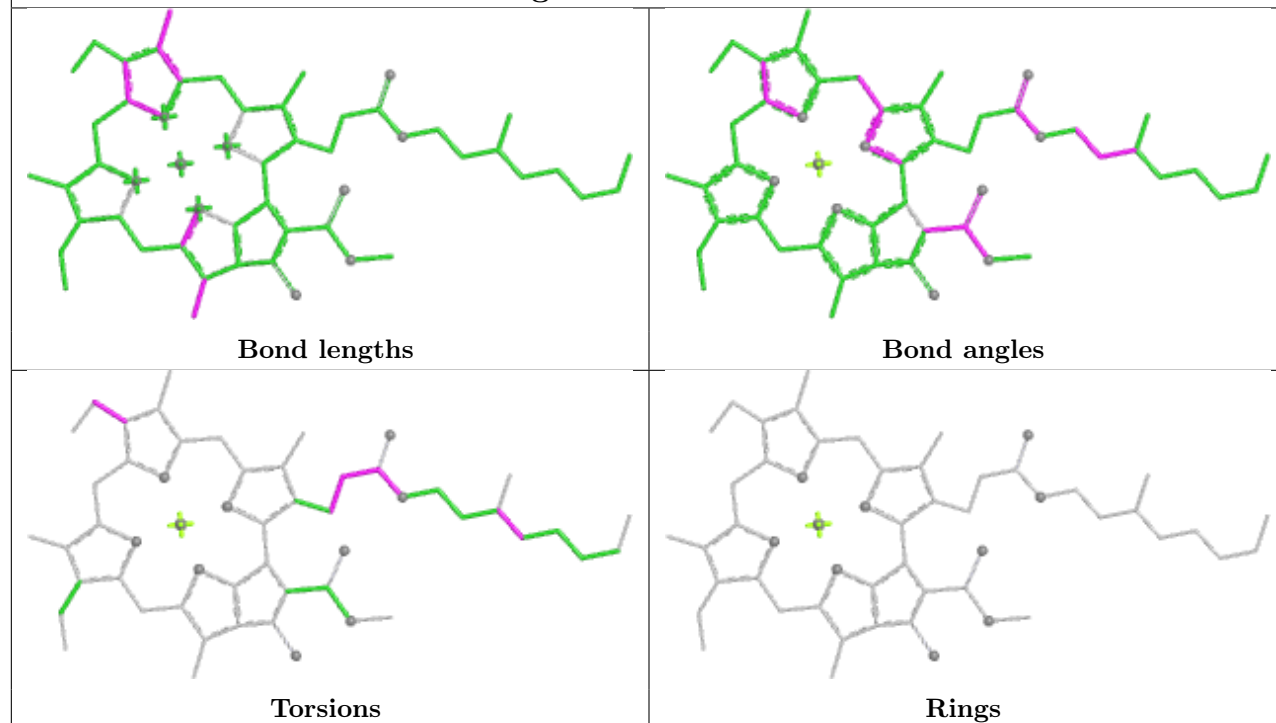
## Ligand LMT a 302



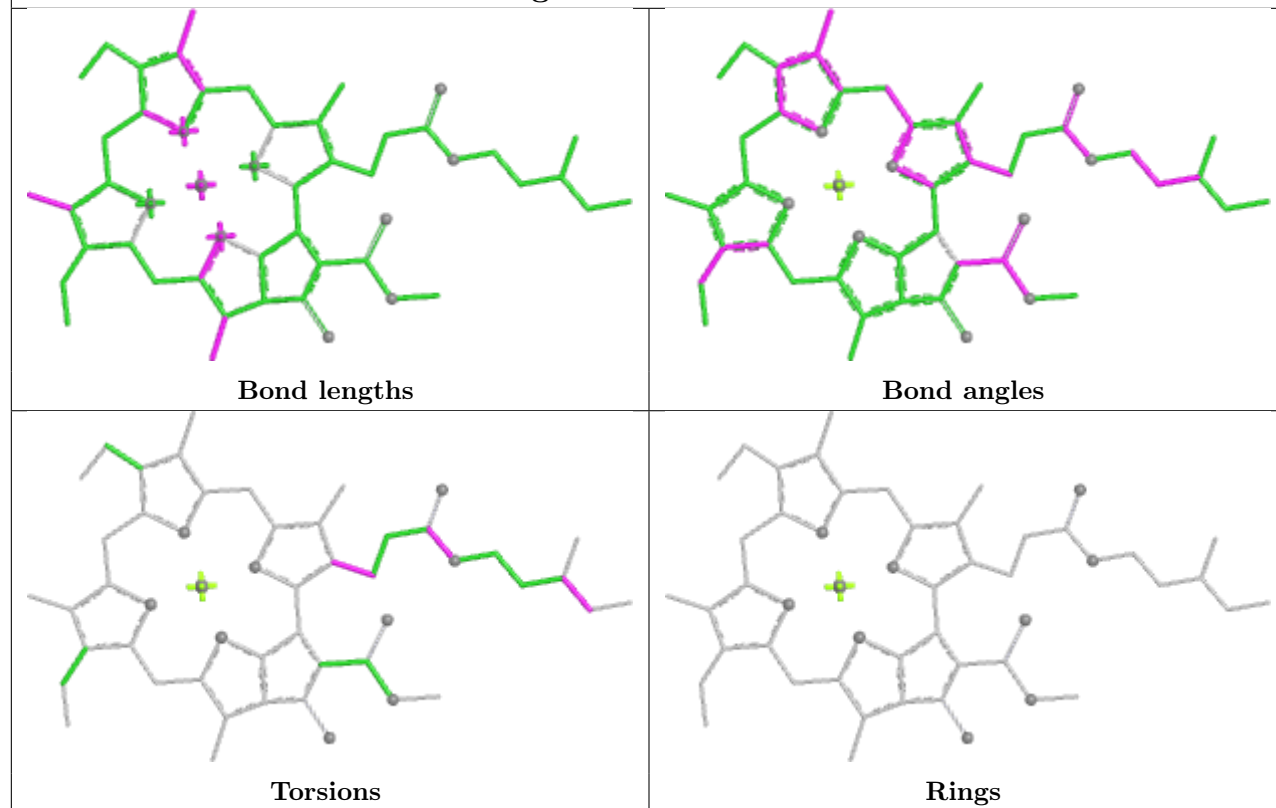


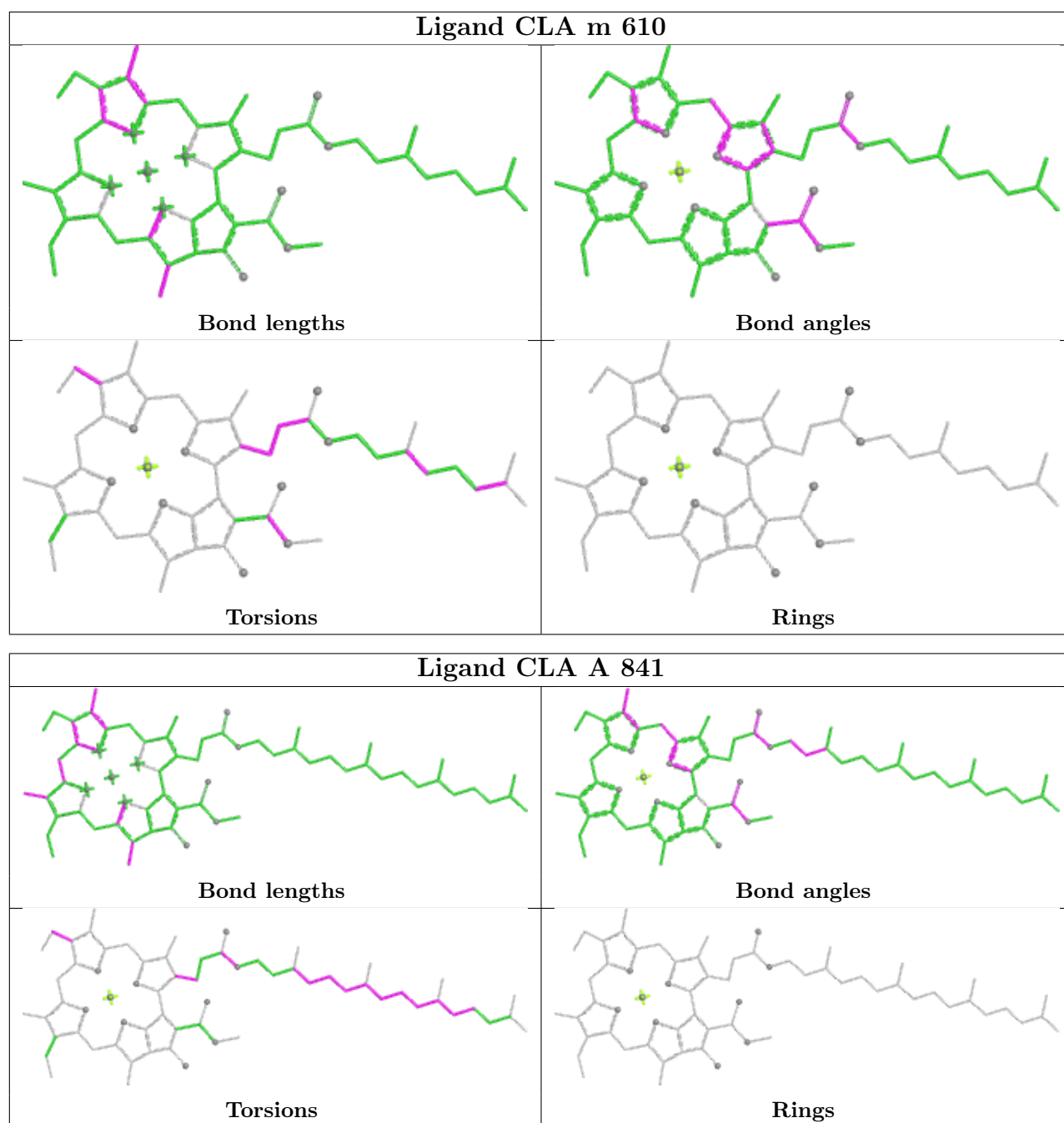
**Ligand CLA B 826****Ligand II0 l 314****Ligand II0 a 316**

## Ligand CLA A 811

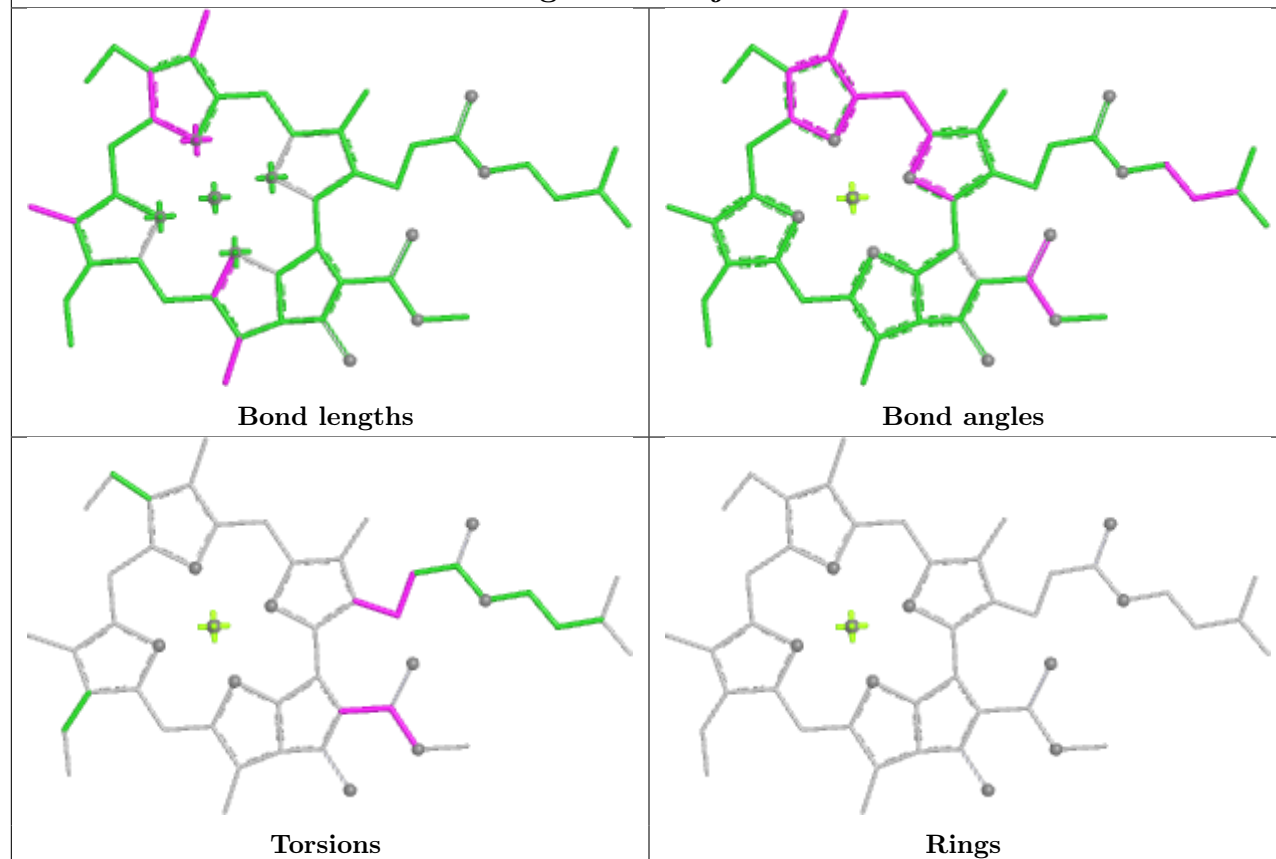


## Ligand CLA A 834

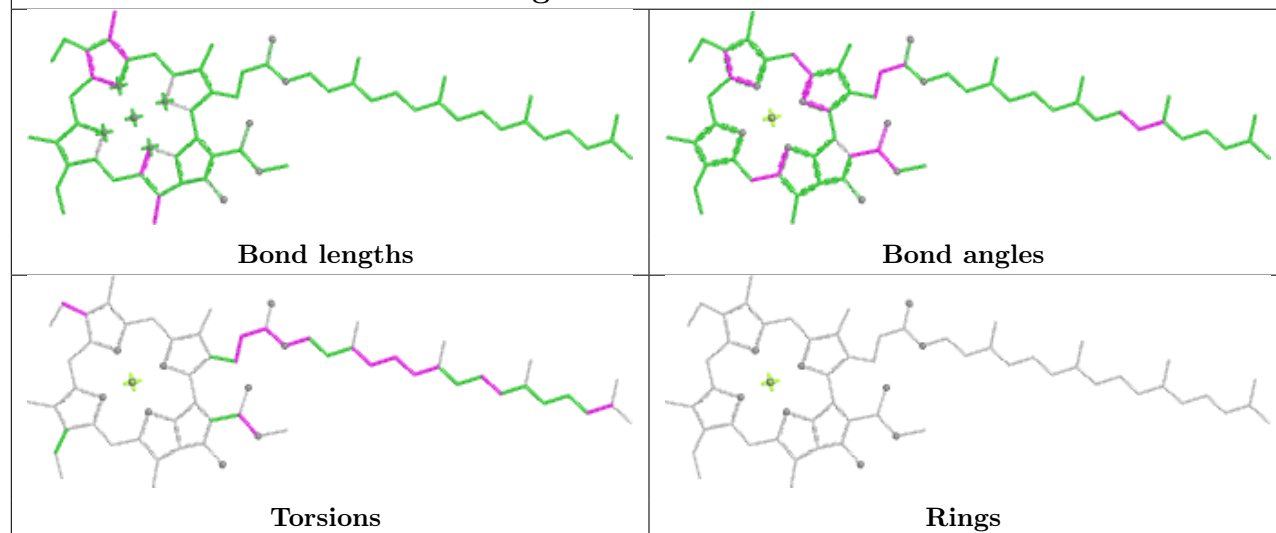


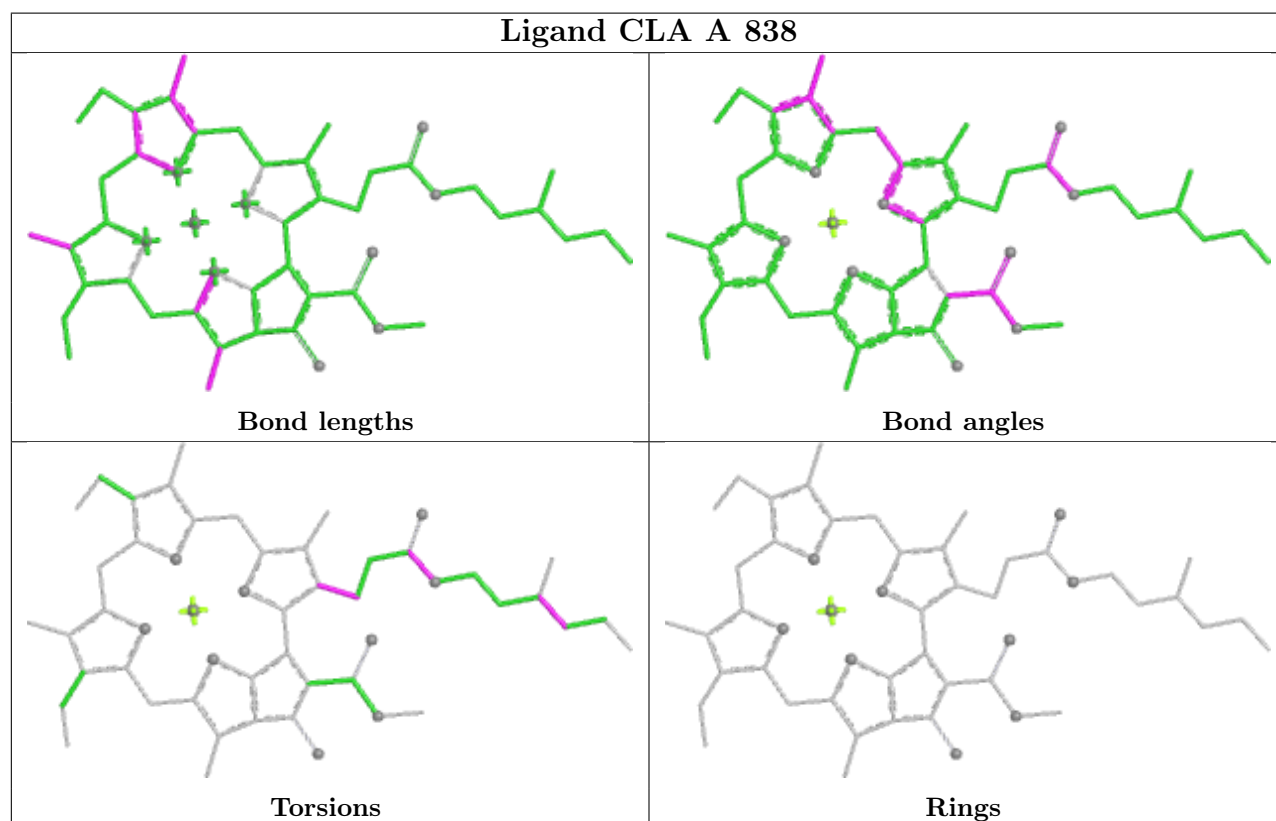
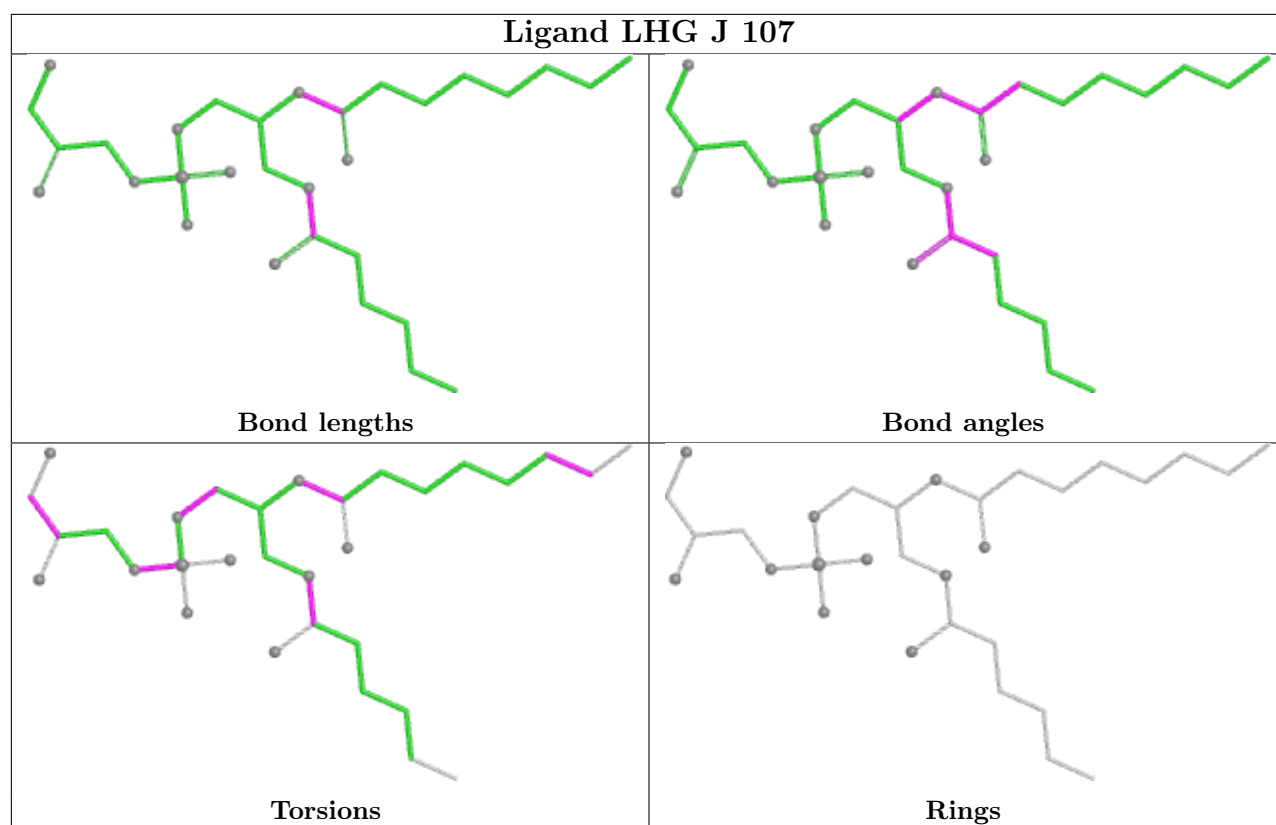


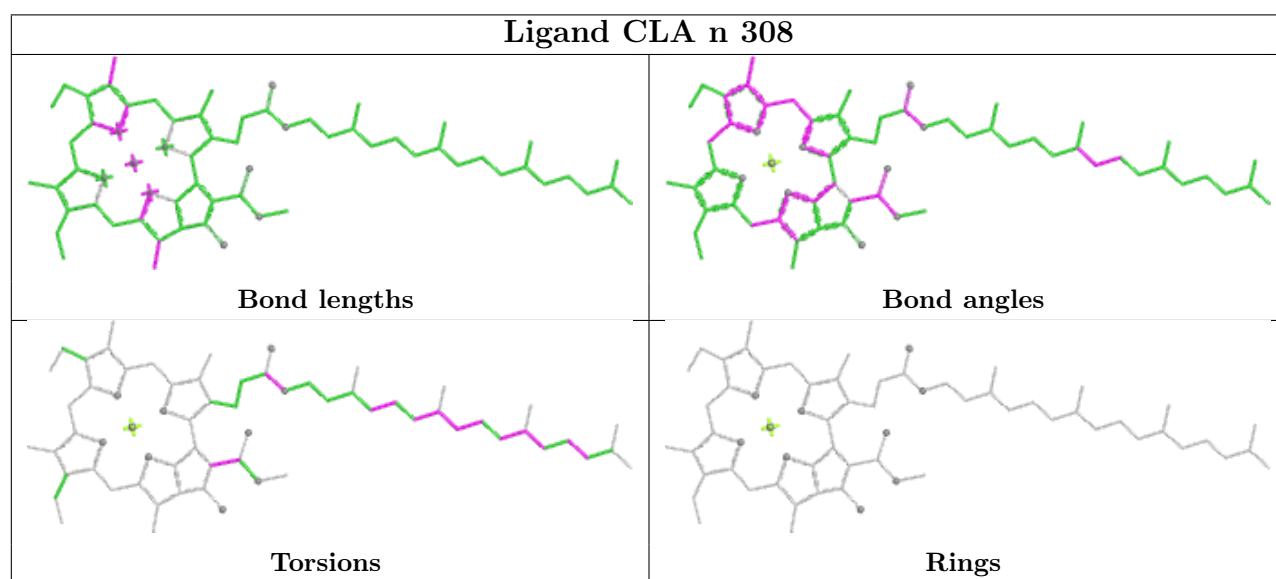
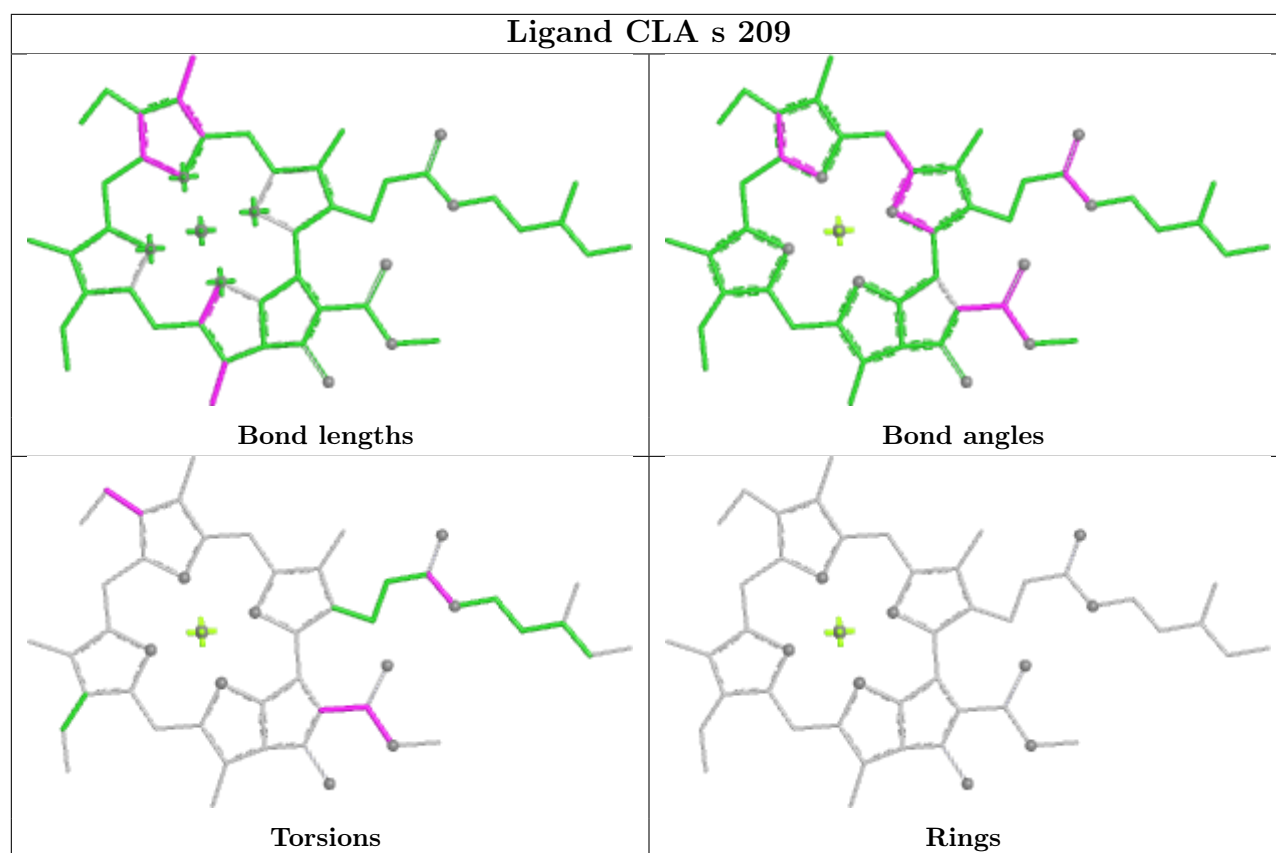
## Ligand CLA j 602

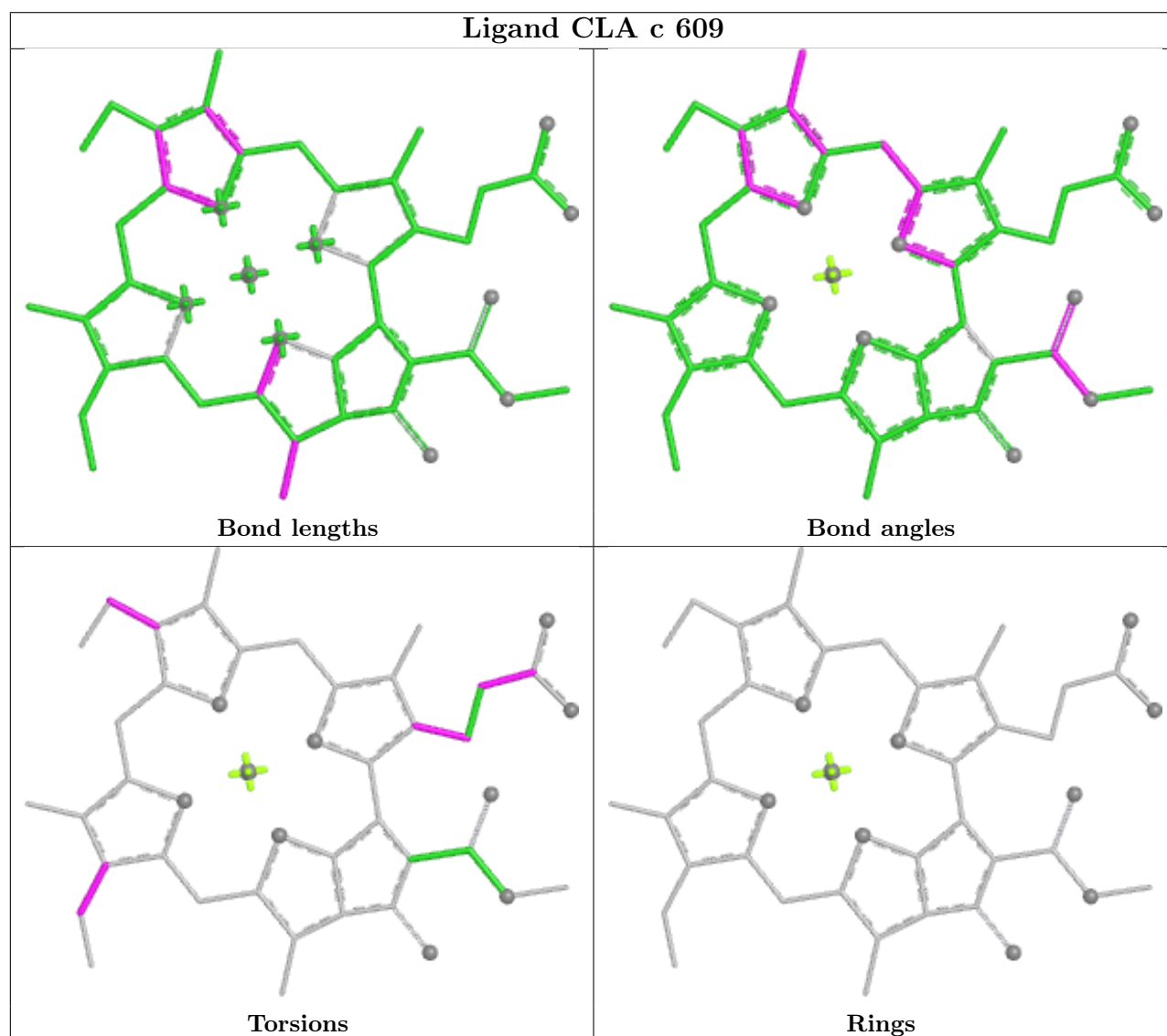
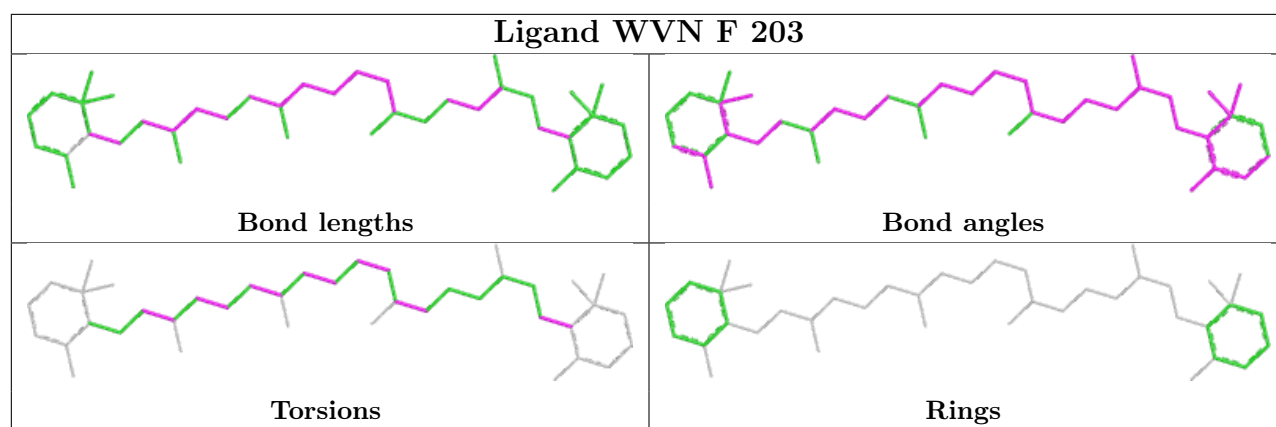


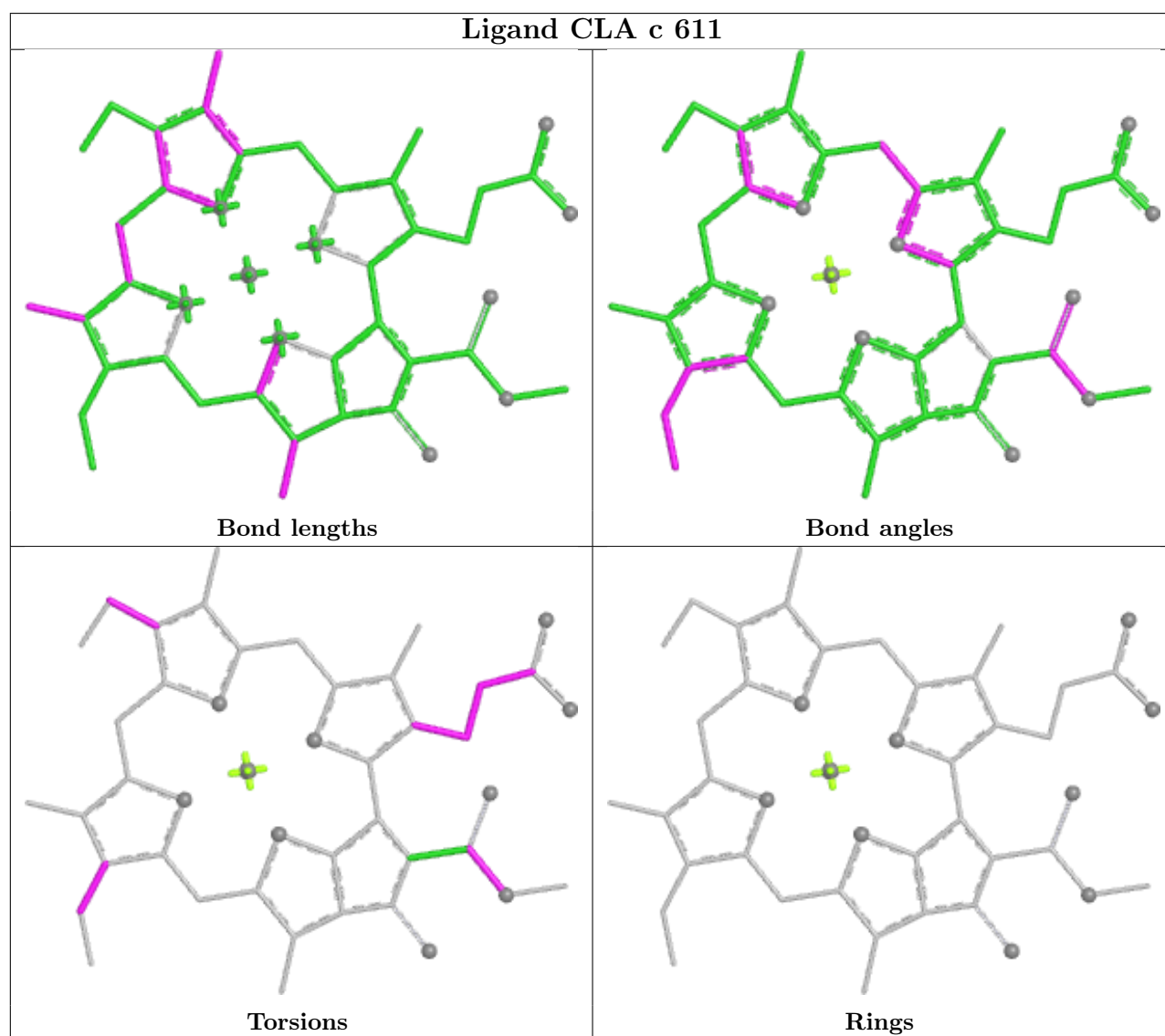
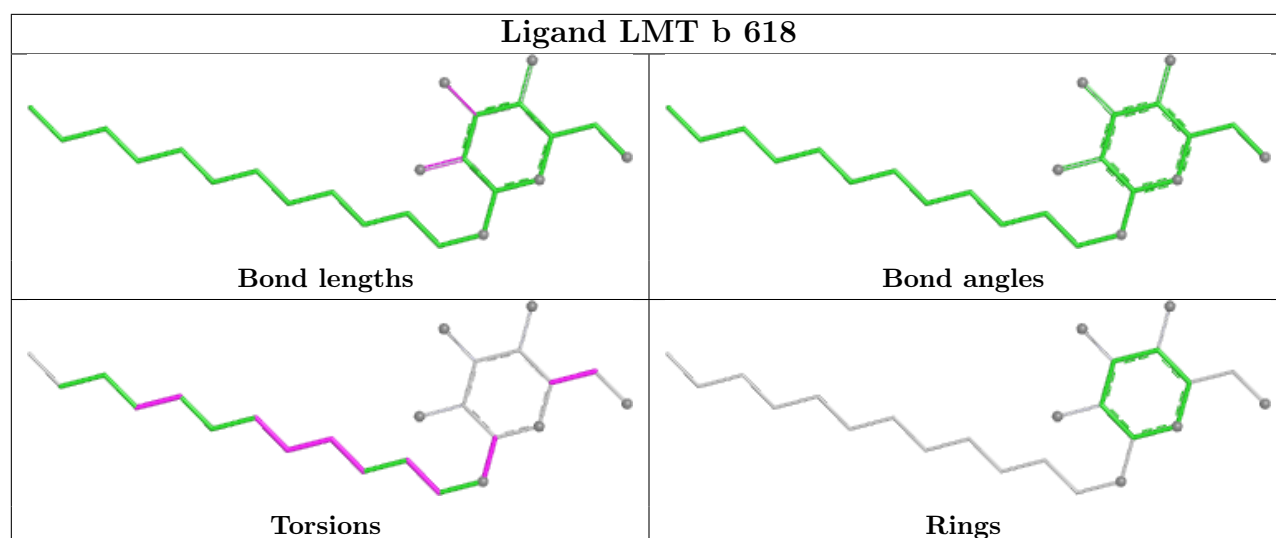
## Ligand CLA B 830



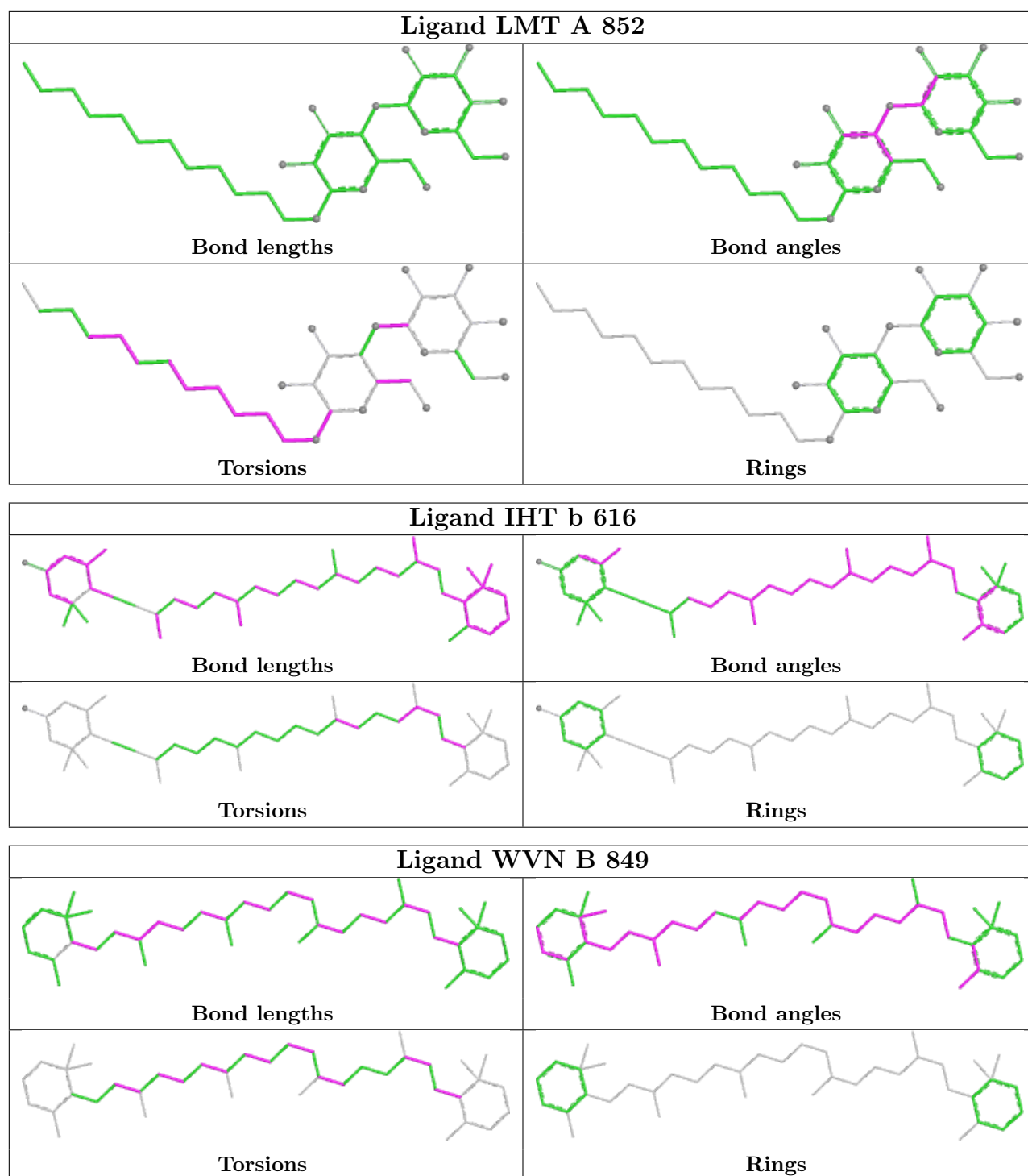




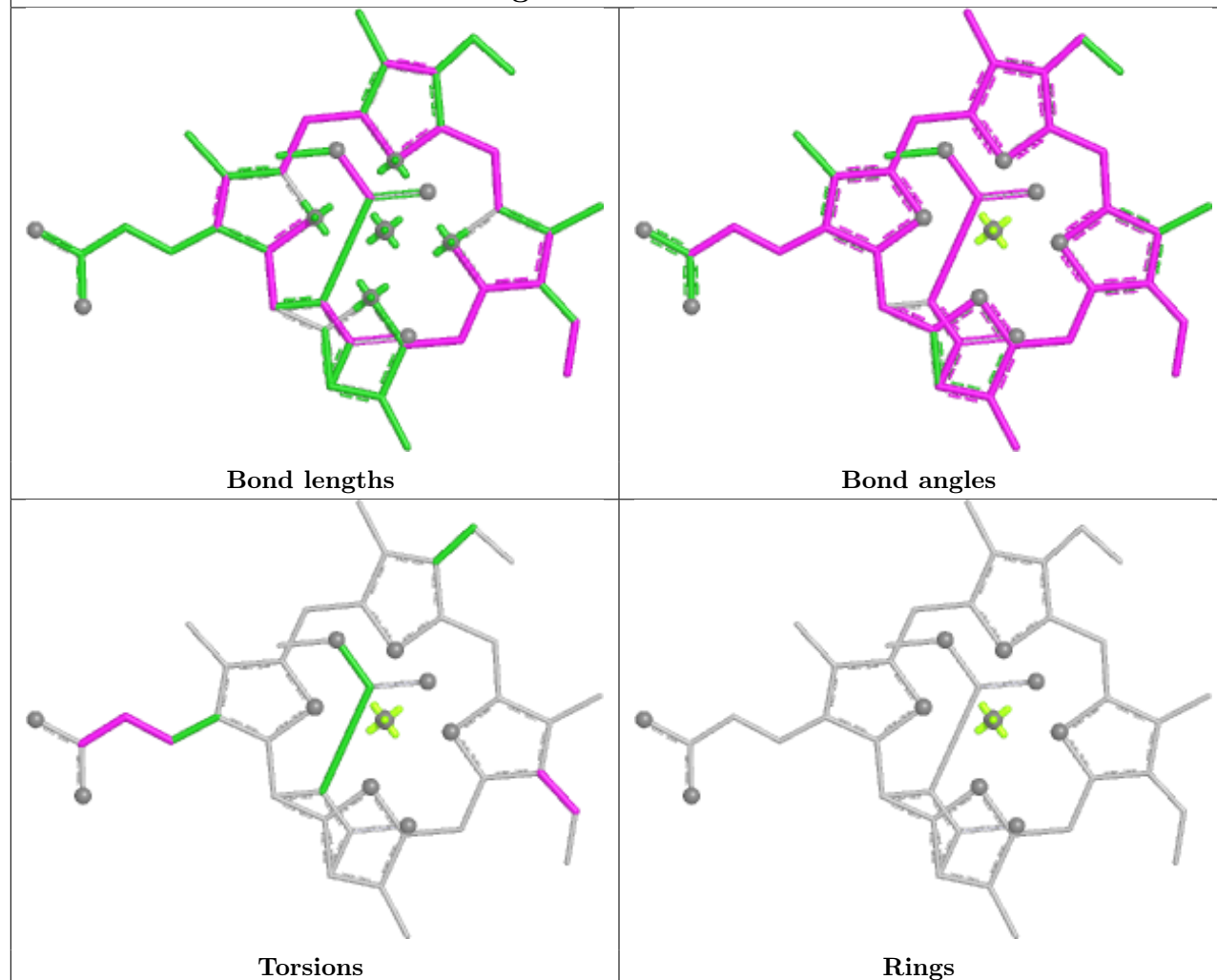




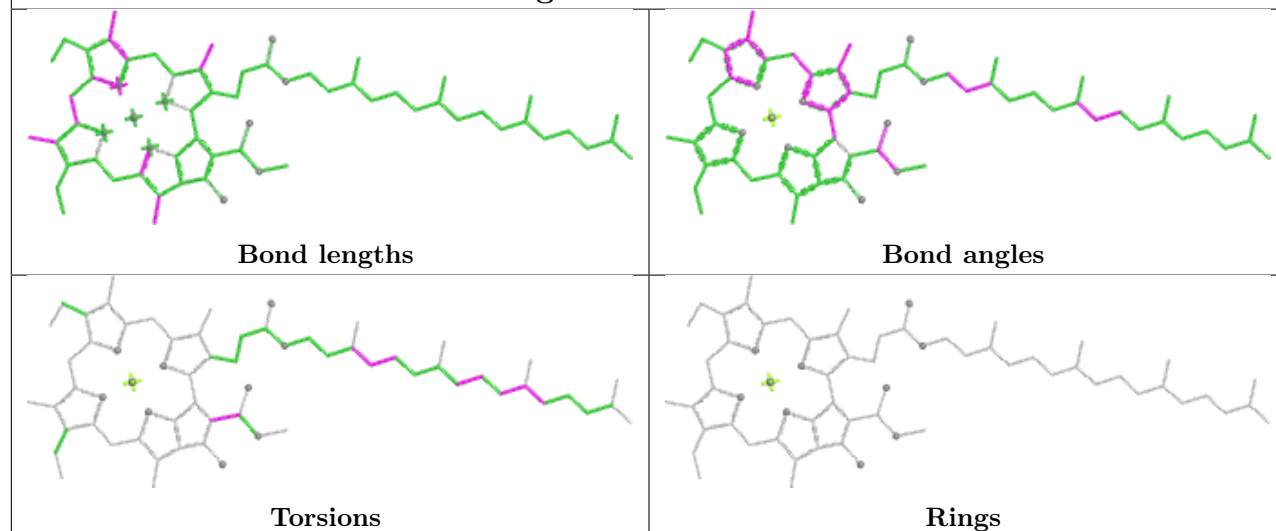


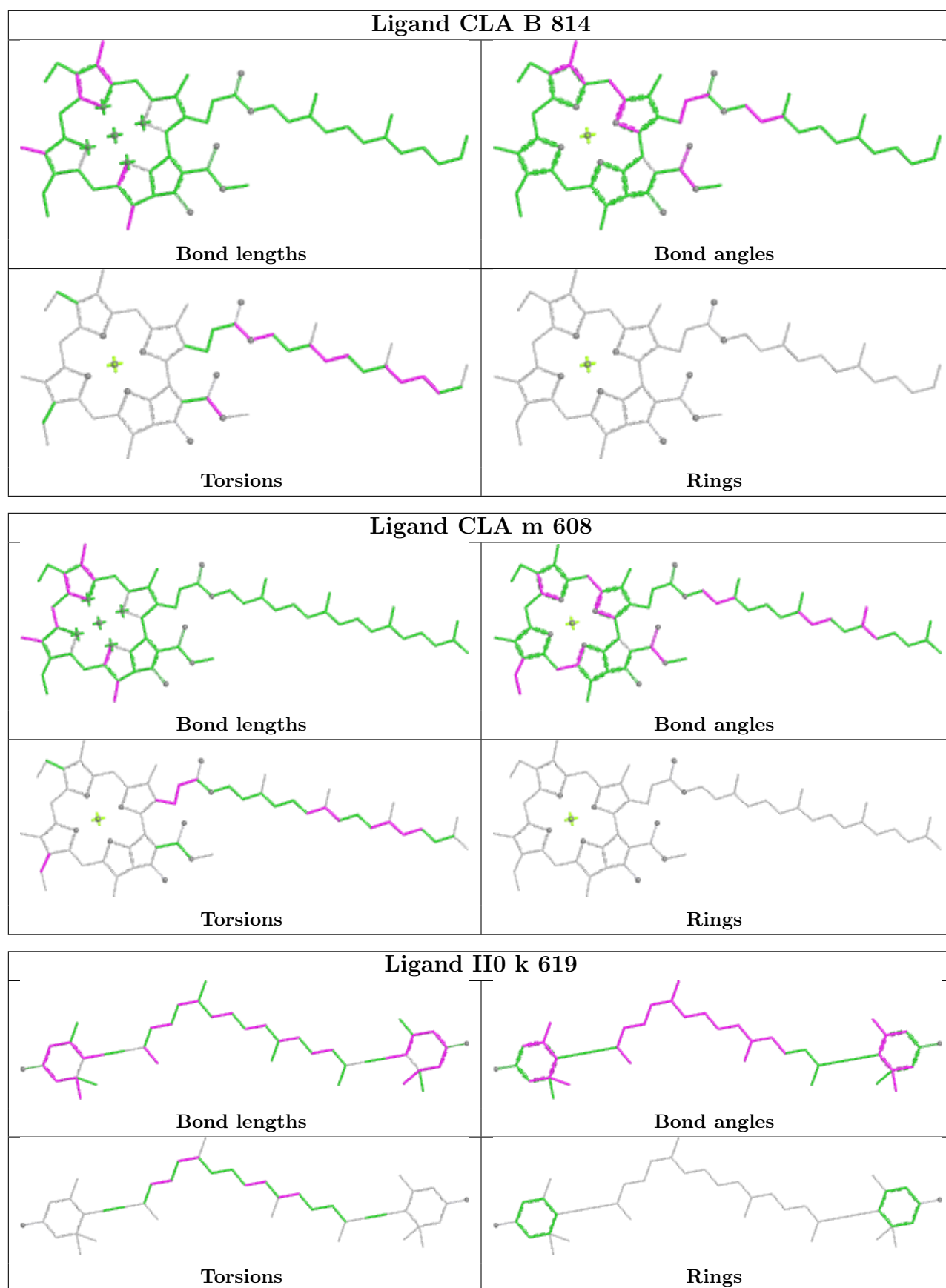


## Ligand KC2 n 312



## Ligand CLA a 309





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37654. These allow visual inspection of the internal detail of the map and identification of artifacts.

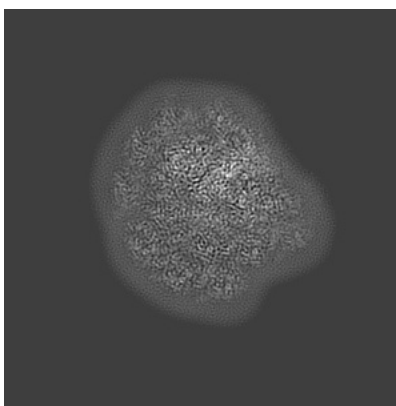
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

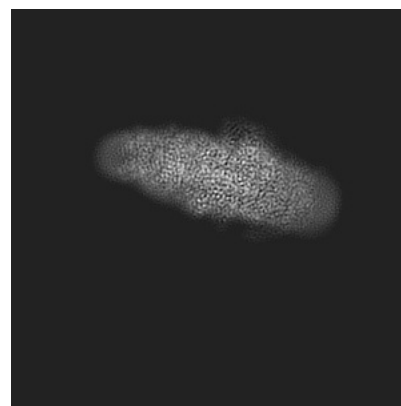
#### 6.1.1 Primary map



X

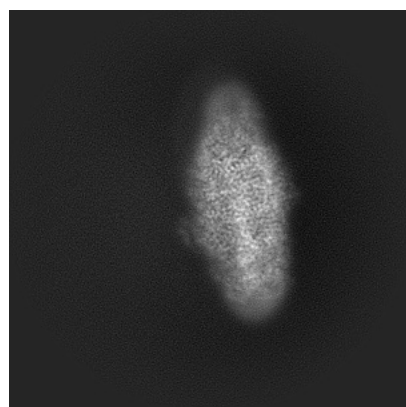


Y

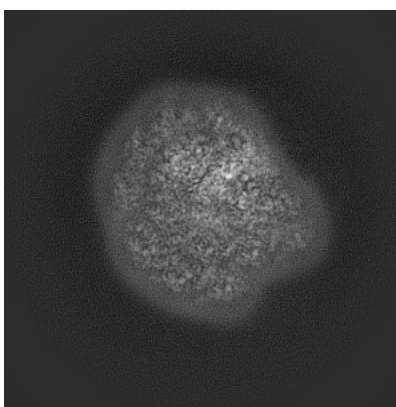


Z

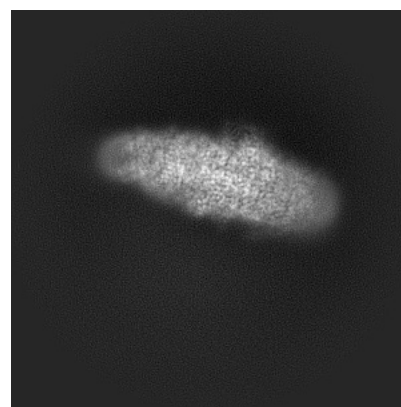
#### 6.1.2 Raw map



X



Y

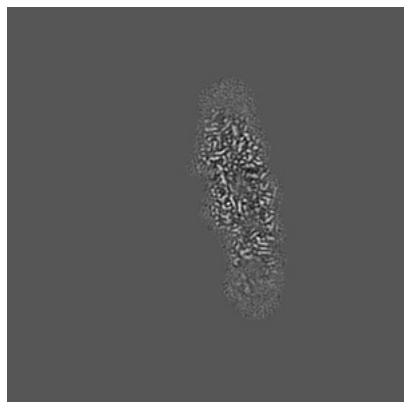


Z

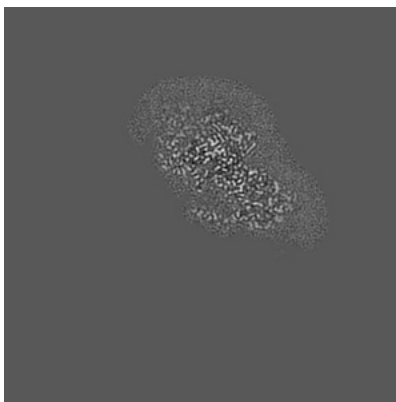
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

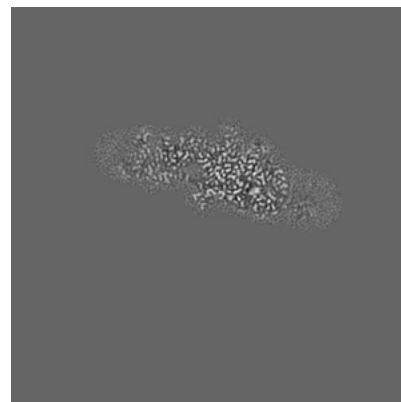
### 6.2.1 Primary map



X Index: 180

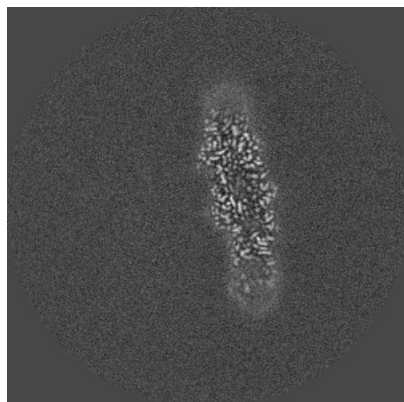


Y Index: 180

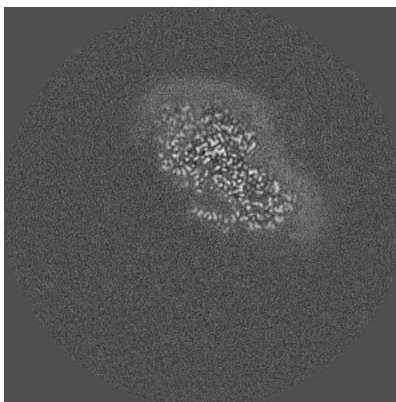


Z Index: 180

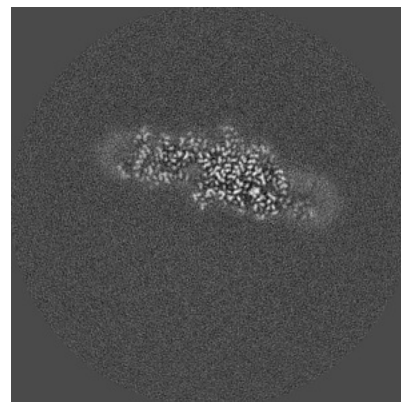
### 6.2.2 Raw map



X Index: 180



Y Index: 180

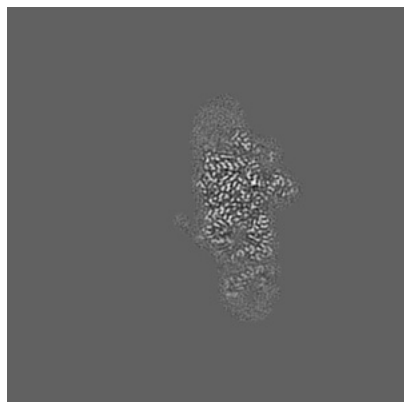


Z Index: 180

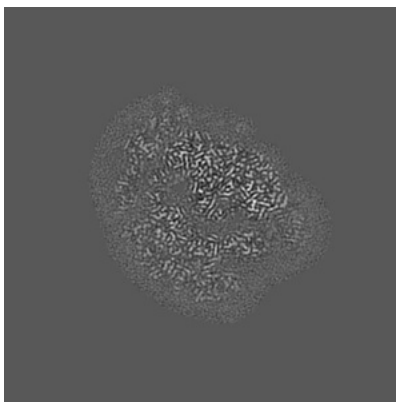
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

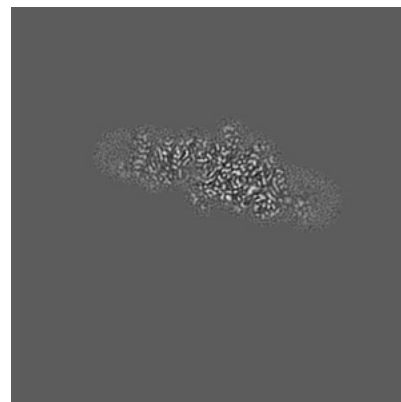
### 6.3.1 Primary map



X Index: 210

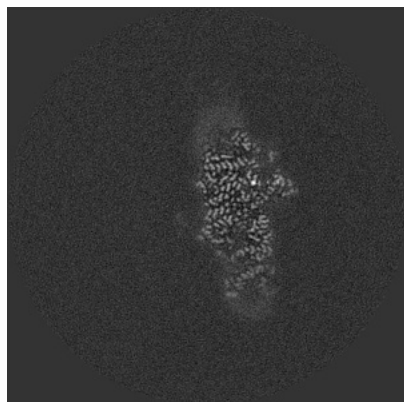


Y Index: 214

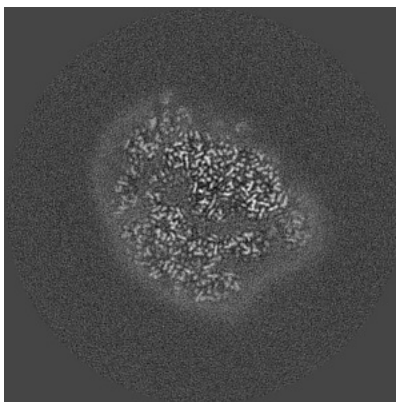


Z Index: 181

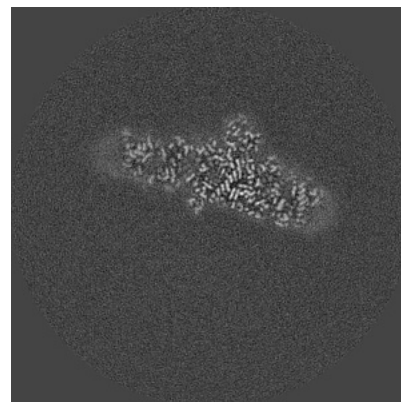
### 6.3.2 Raw map



X Index: 210



Y Index: 214



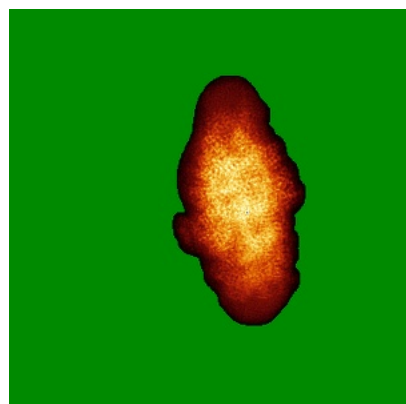
Z Index: 195

The images above show the largest variance slices of the map in three orthogonal directions.

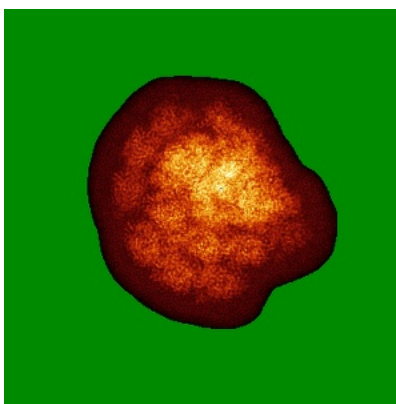


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

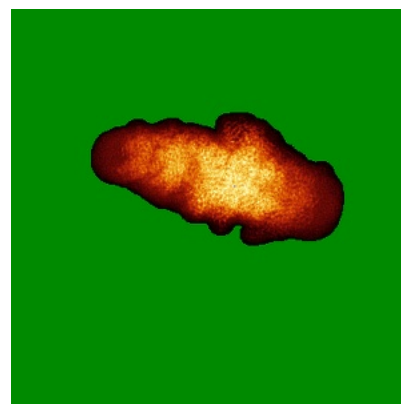
### 6.4.1 Primary map



X

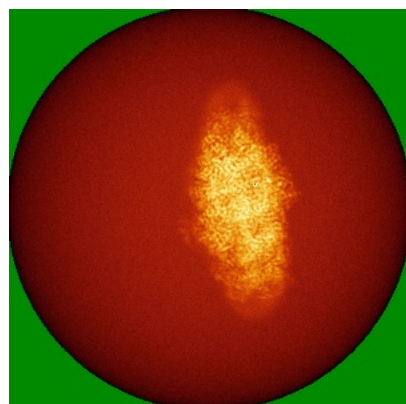


Y

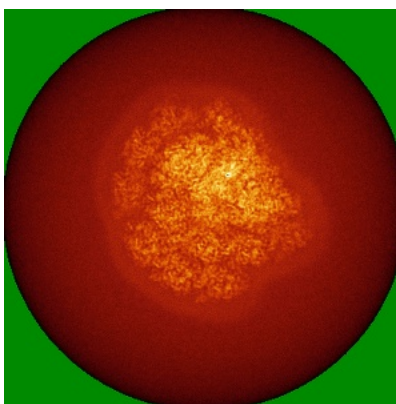


Z

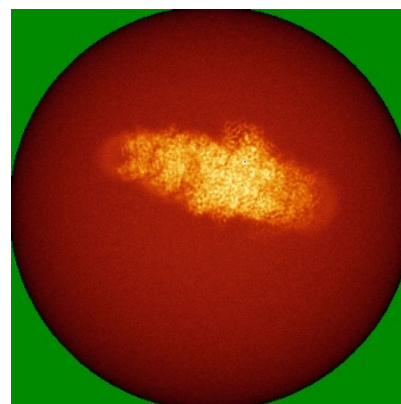
### 6.4.2 Raw map



X



Y



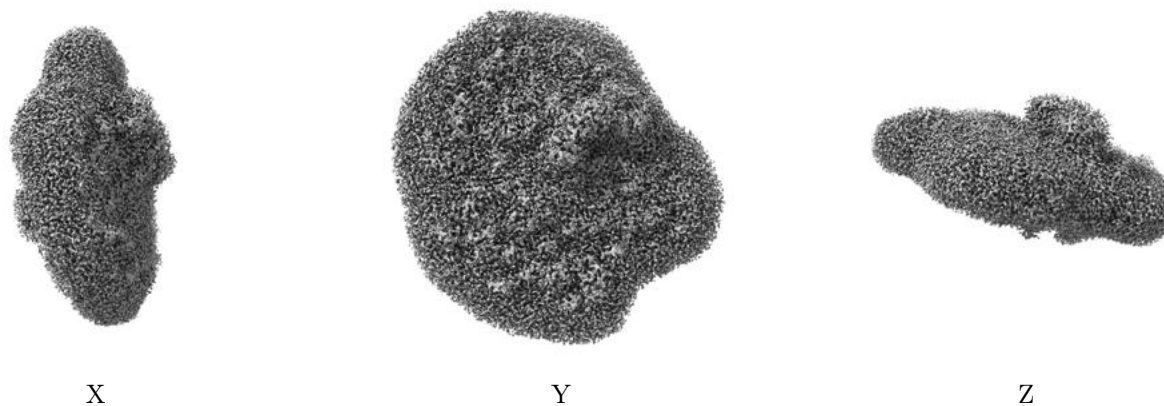
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



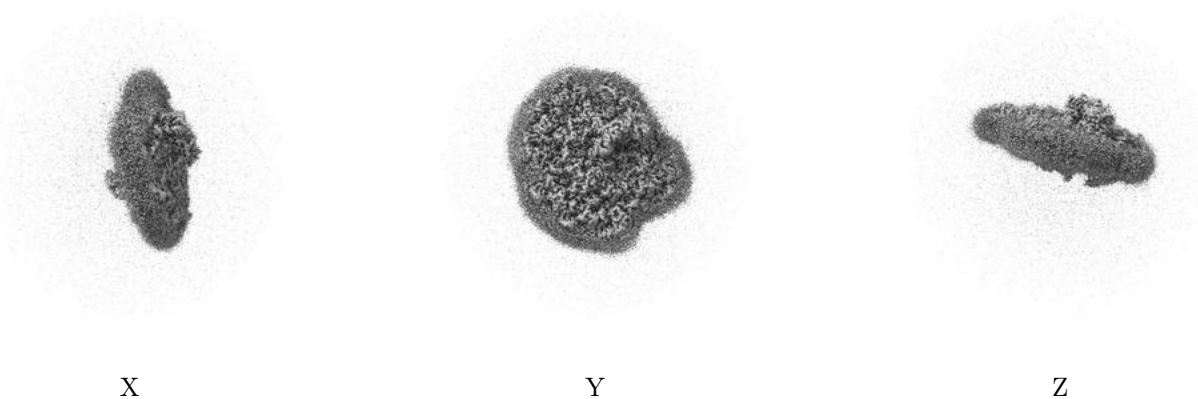
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

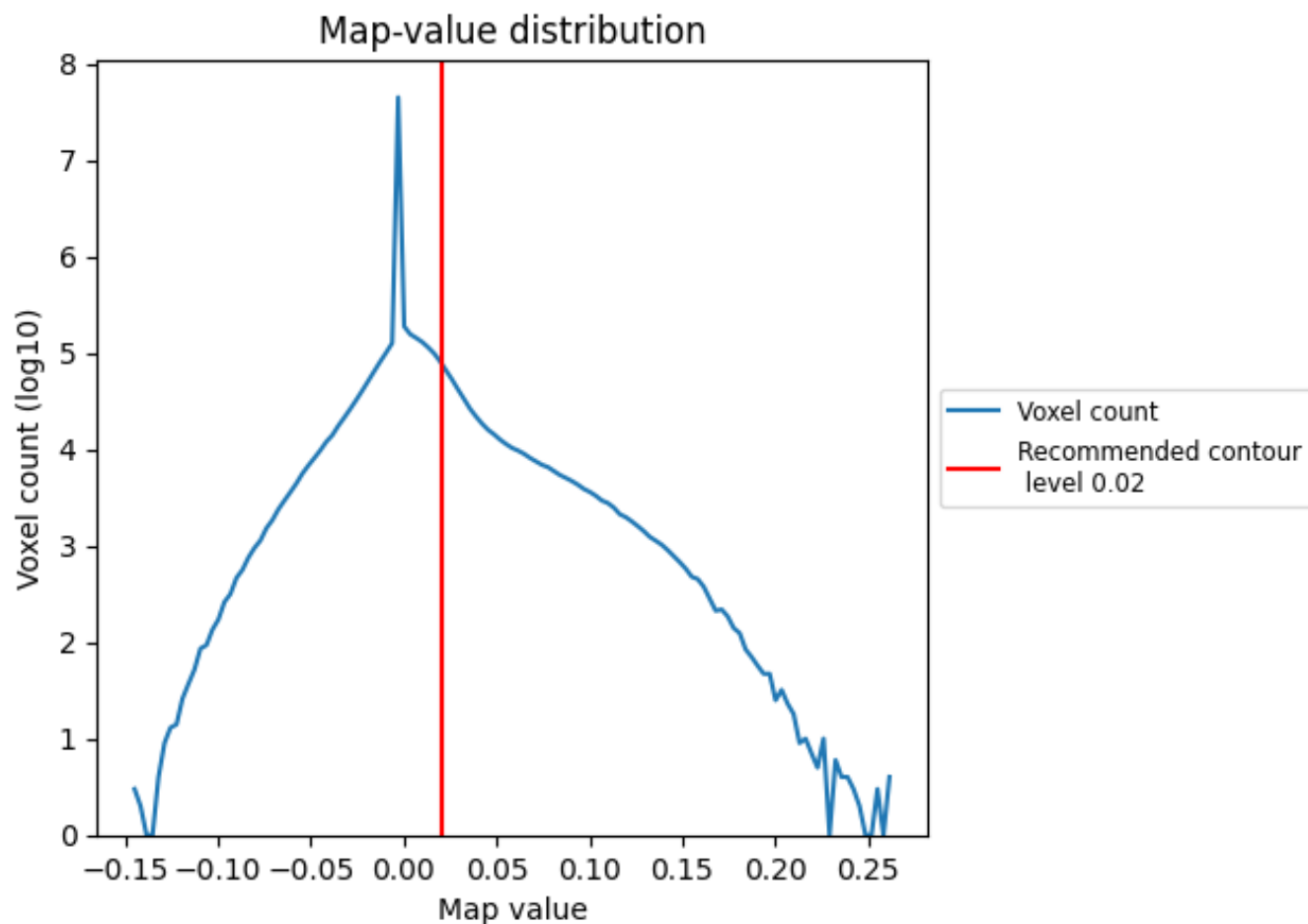
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

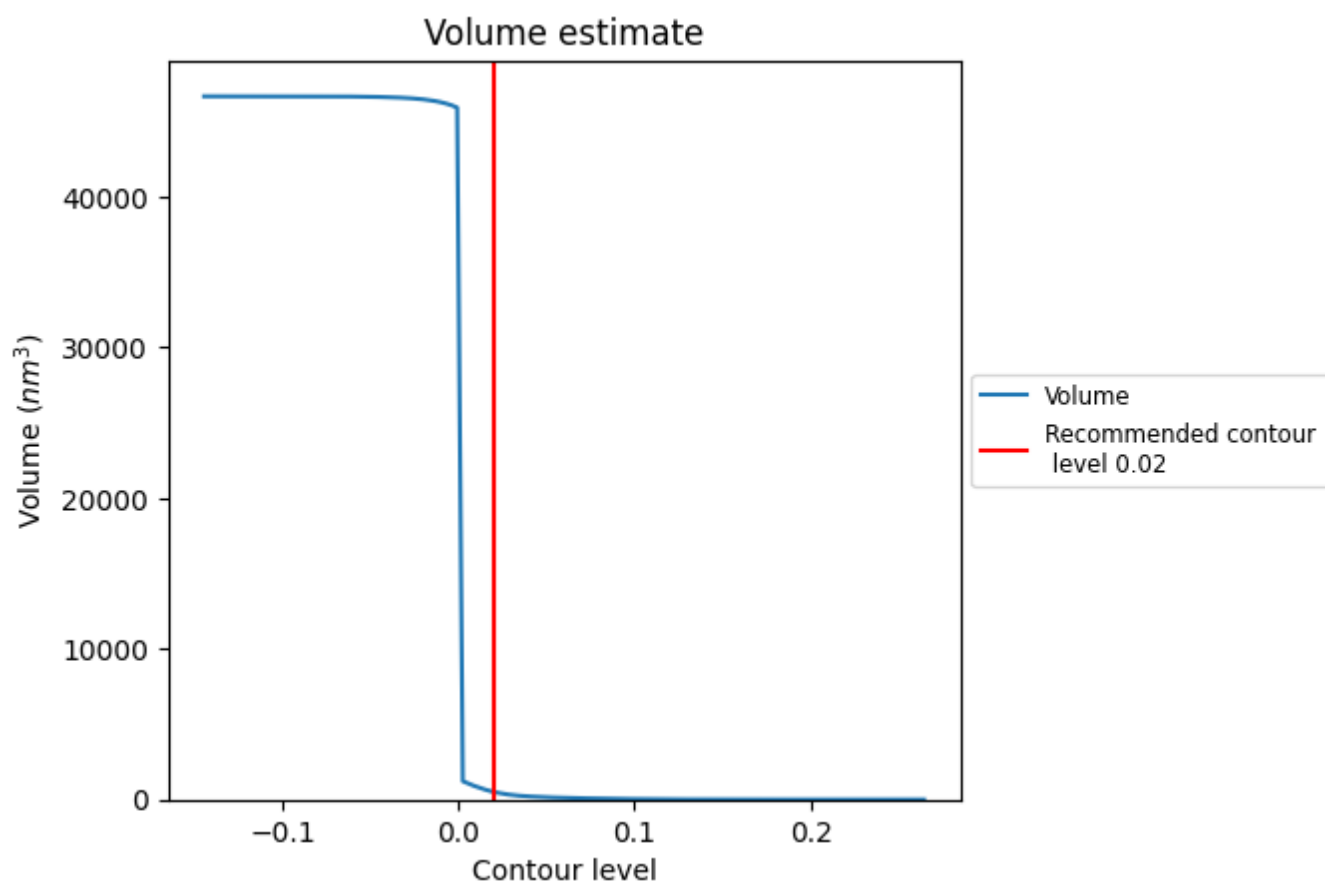
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

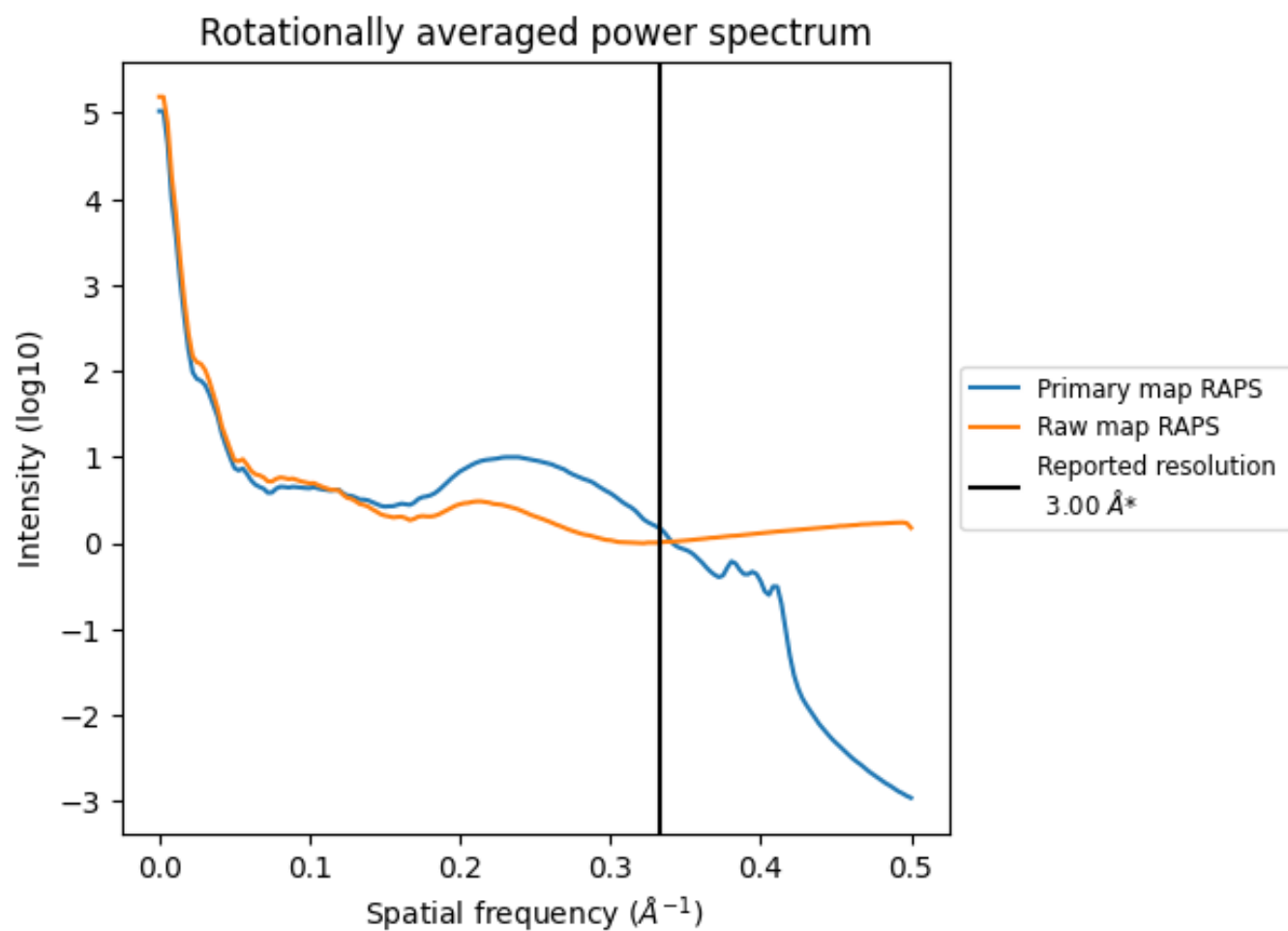
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 508 nm<sup>3</sup>; this corresponds to an approximate mass of 459 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

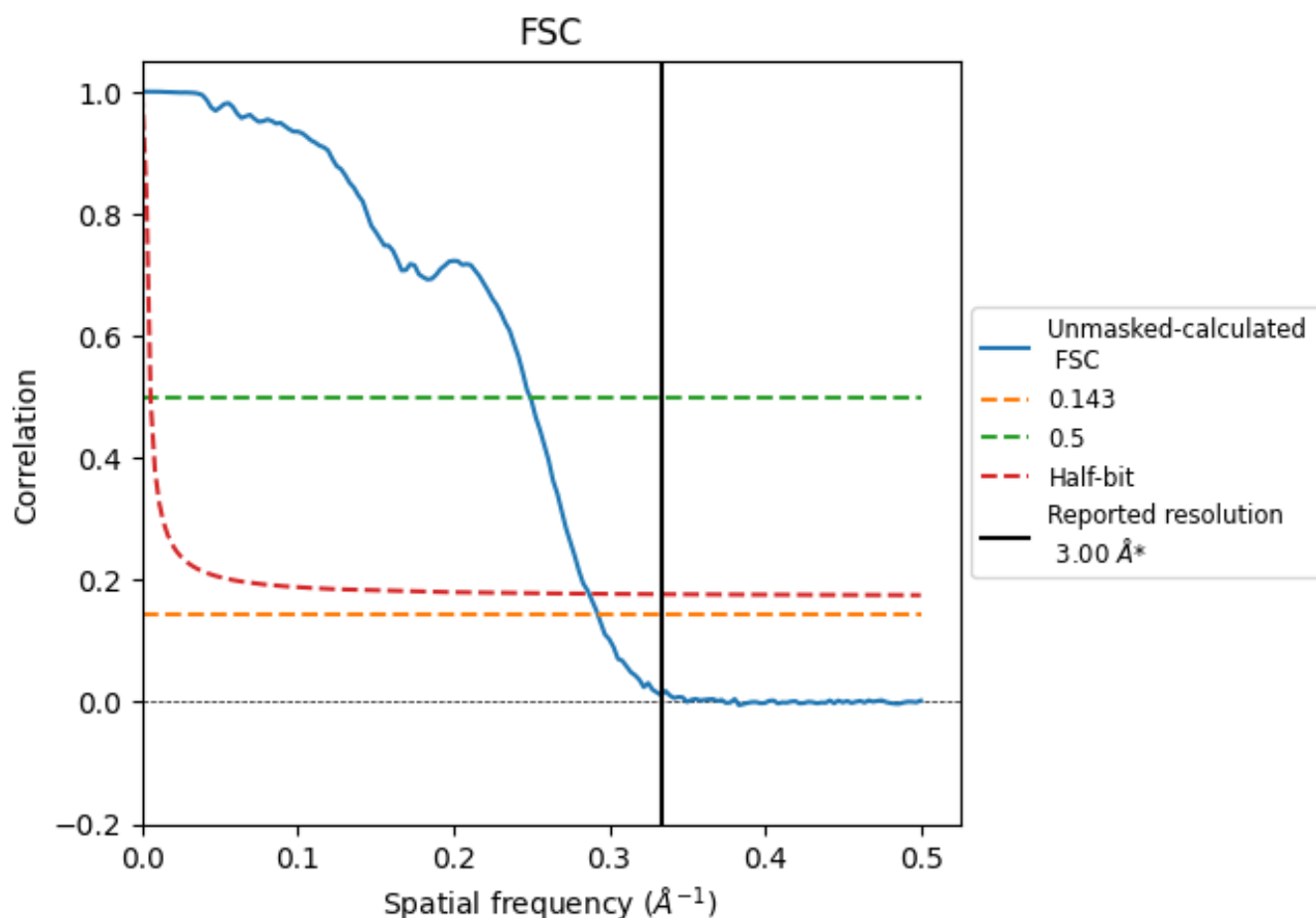


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

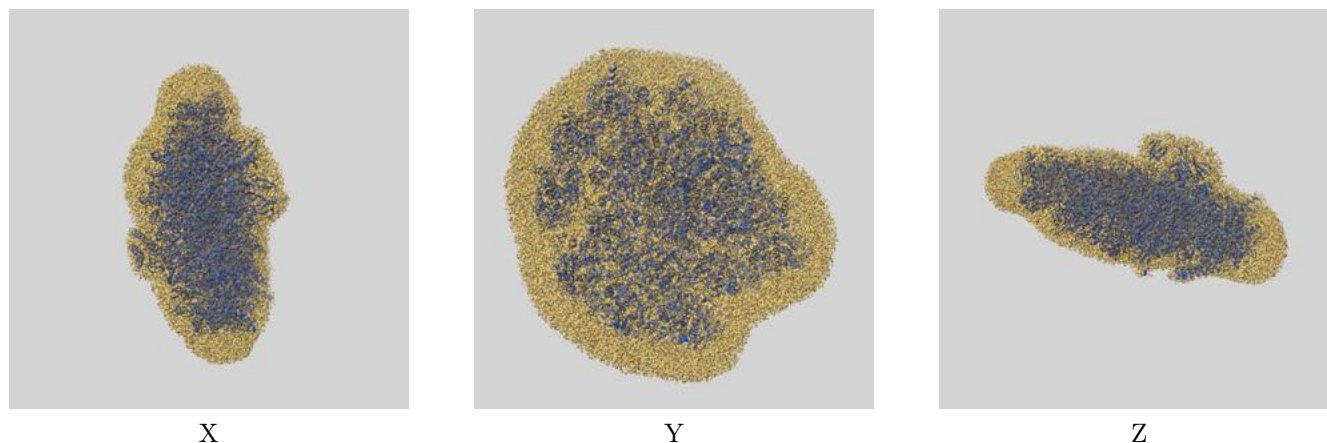
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.00                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.42                               | 4.01 | 3.48     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.0 by more than 10 %

## 9 Map-model fit [i](#)

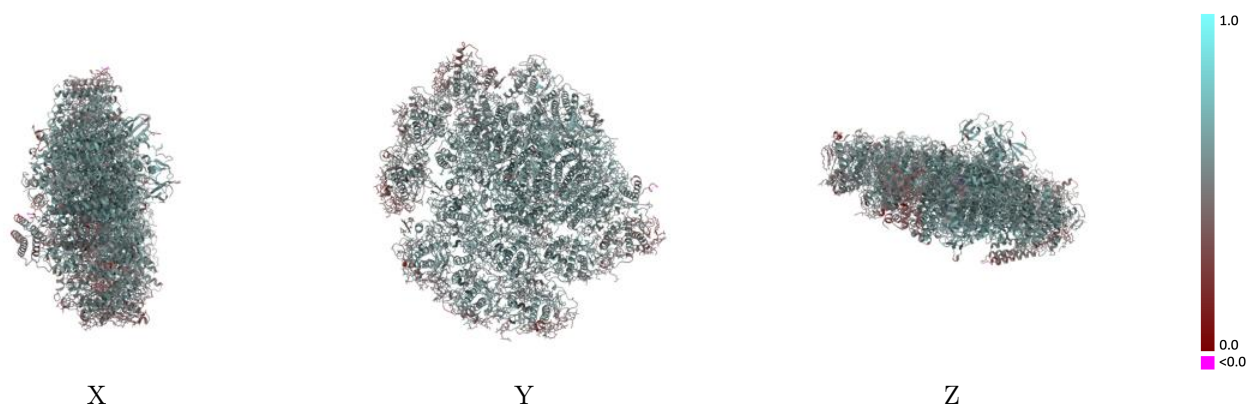
This section contains information regarding the fit between EMDB map EMD-37654 and PDB model 8WMJ. Per-residue inclusion information can be found in section [3](#) on page [35](#).

### 9.1 Map-model overlay [i](#)



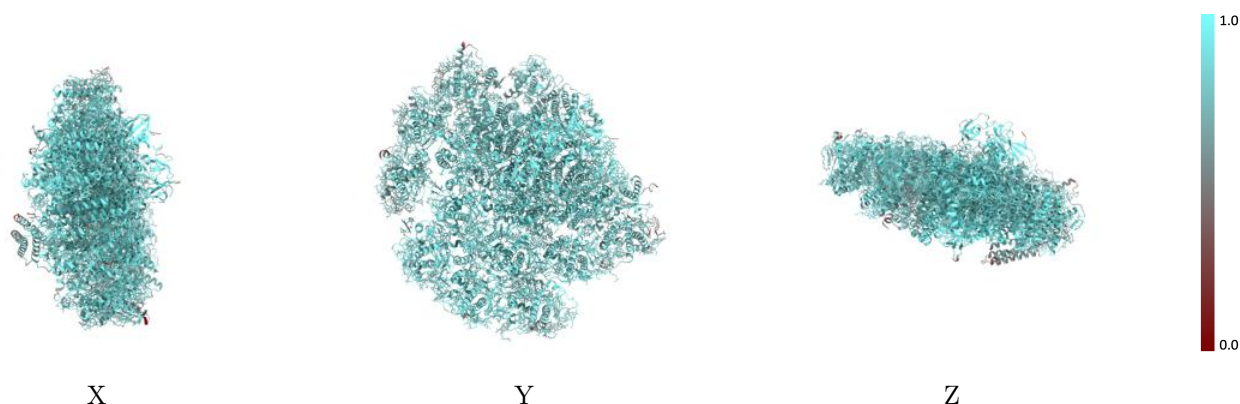
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

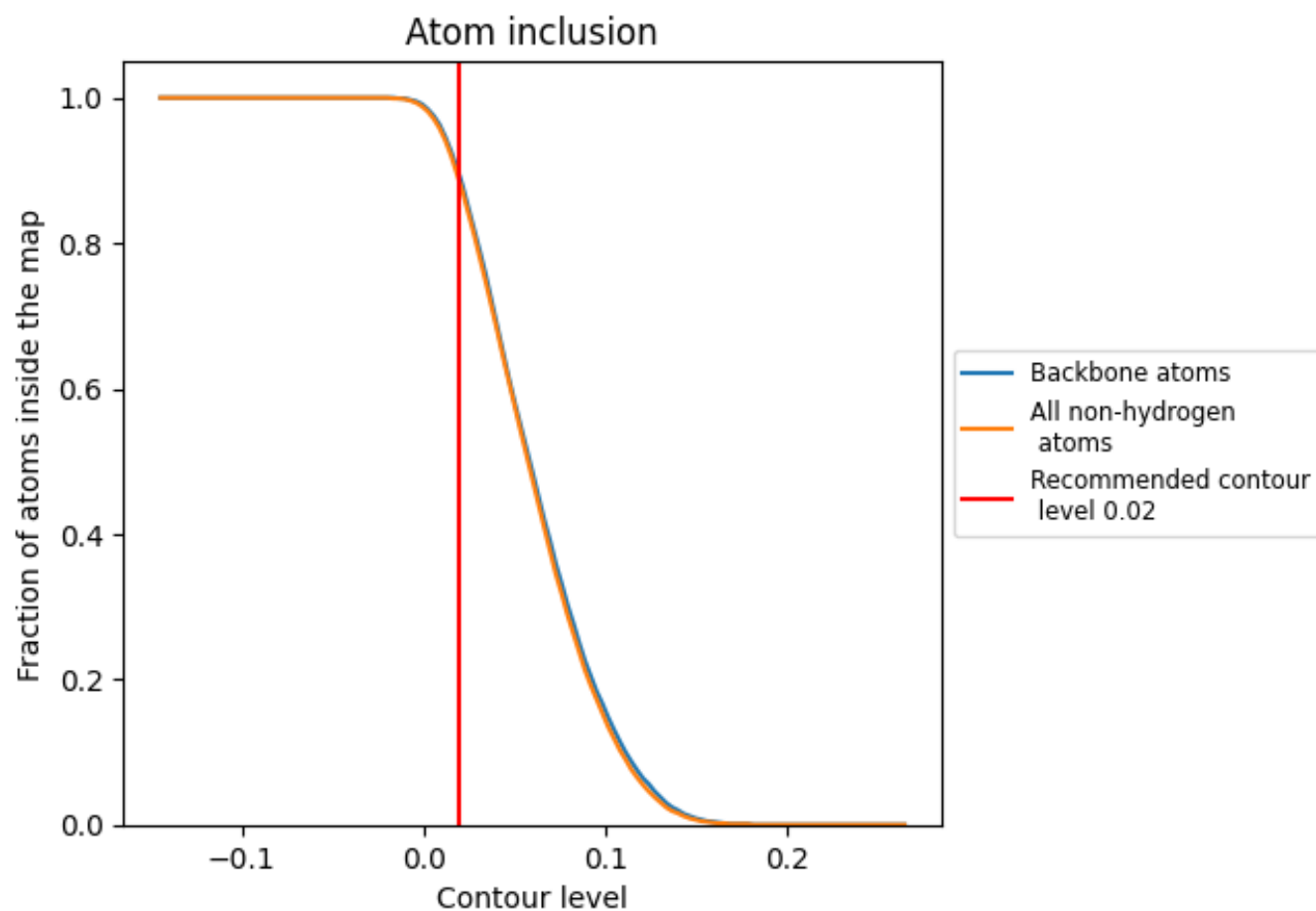
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8830   |  0.5530   |
| A     |  0.9460   |  0.6100   |
| B     |  0.9530   |  0.6120   |
| C     |  0.9410   |  0.5910   |
| D     |  0.8900   |  0.5580   |
| E     |  0.8850   |  0.5500   |
| F     |  0.9220   |  0.5840   |
| I     |  0.8940   |  0.5780   |
| J     |  0.9300   |  0.5920   |
| K     |  0.8240   |  0.5130   |
| L     |  0.8430   |  0.5350   |
| M     |  0.8910   |  0.5650   |
| Q     |  0.6840   |  0.4300   |
| R     |  0.9010   |  0.5660   |
| a     |  0.9300  |  0.5780  |
| b     |  0.9160 |  0.5800 |
| c     |  0.8770 |  0.5500 |
| d     |  0.7380 |  0.4250 |
| h     |  0.8570 |  0.5310 |
| i     |  0.7650 |  0.4540 |
| j     |  0.8170 |  0.4980 |
| k     |  0.7670 |  0.4580 |
| l     |  0.8590 |  0.5230 |
| m     |  0.8690 |  0.5300 |
| n     |  0.8230 |  0.5000 |
| s     |  0.9030 |  0.5690 |

